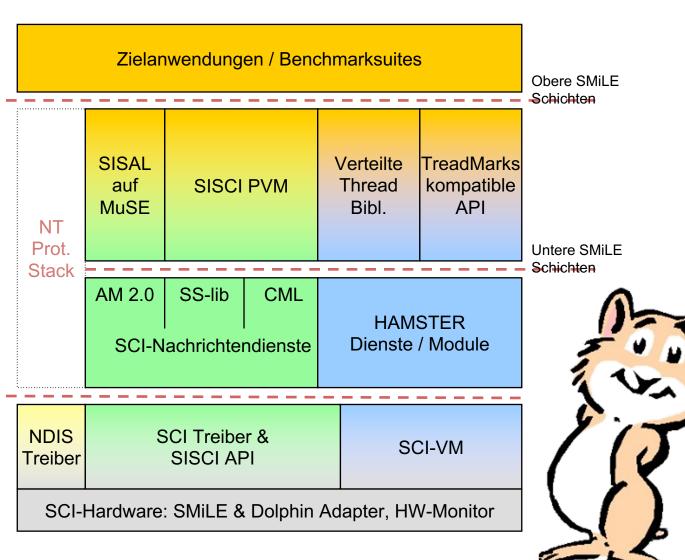


On the Quest for More Performance Martin Schulz @ APART 25th Anniversary Workshop Obergurgl, February 14th, 2024

The Early Days Performance Engineering für SCI

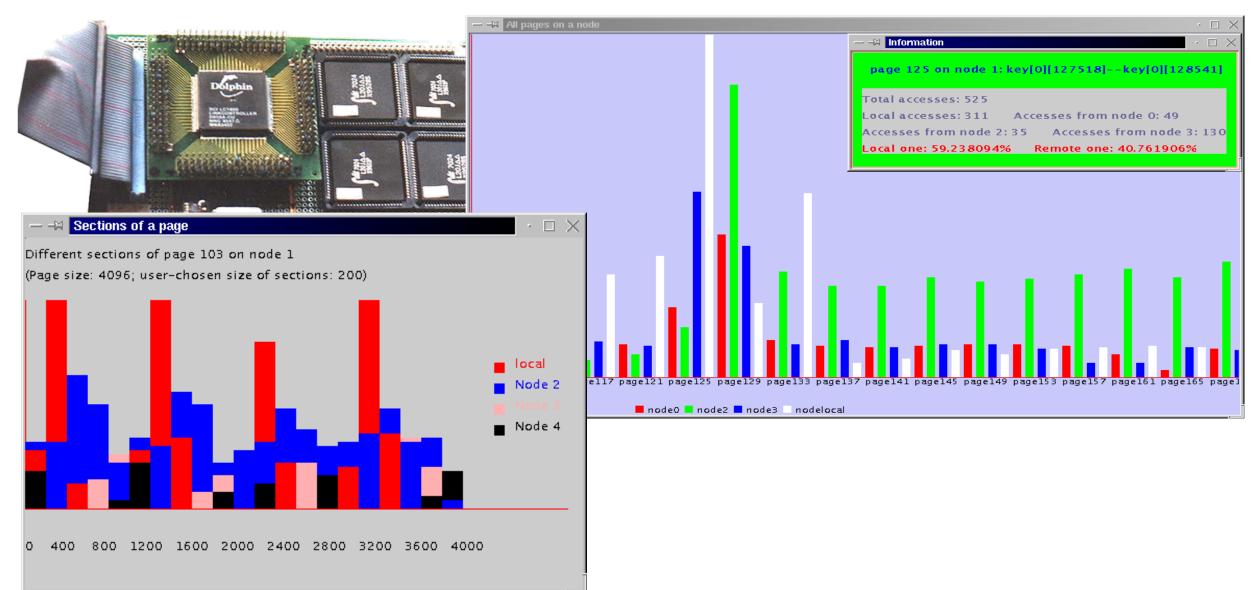




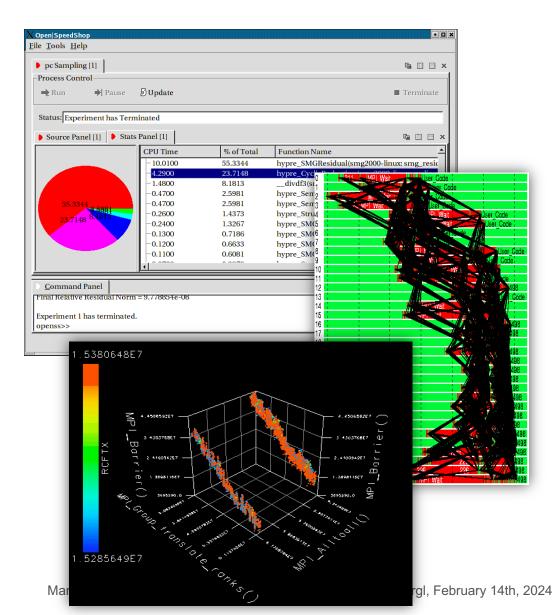


The Early Days Hardware Monitoring and Tools

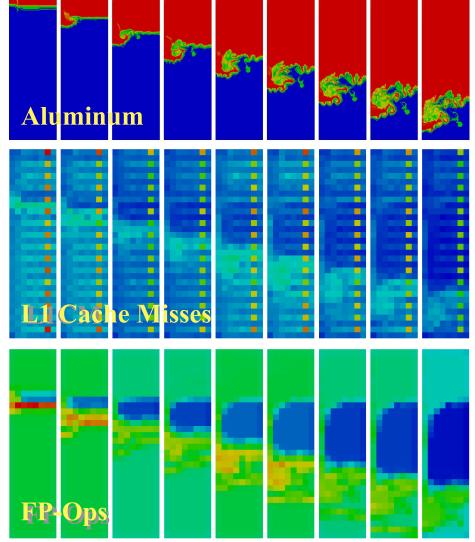




Tools Work at LLNL From Open|SpeedShop to PAVE

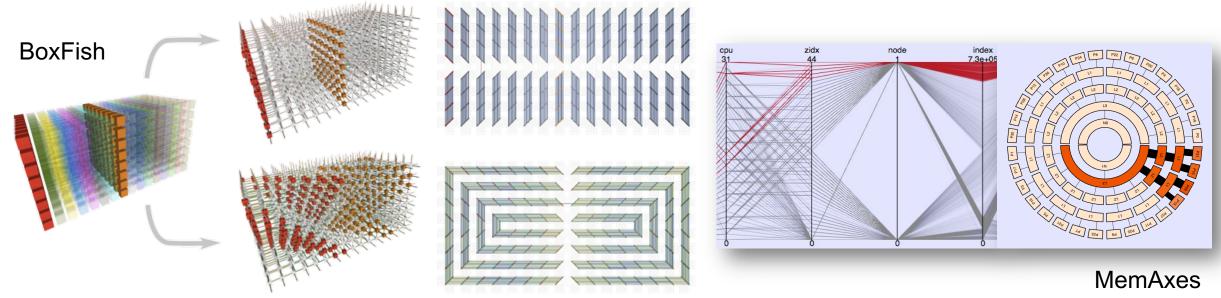




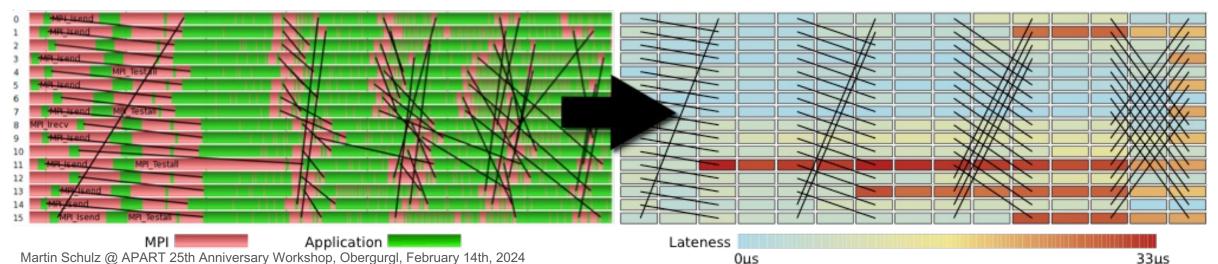


Visual Performance Analysis PAVE Tools





Ravel



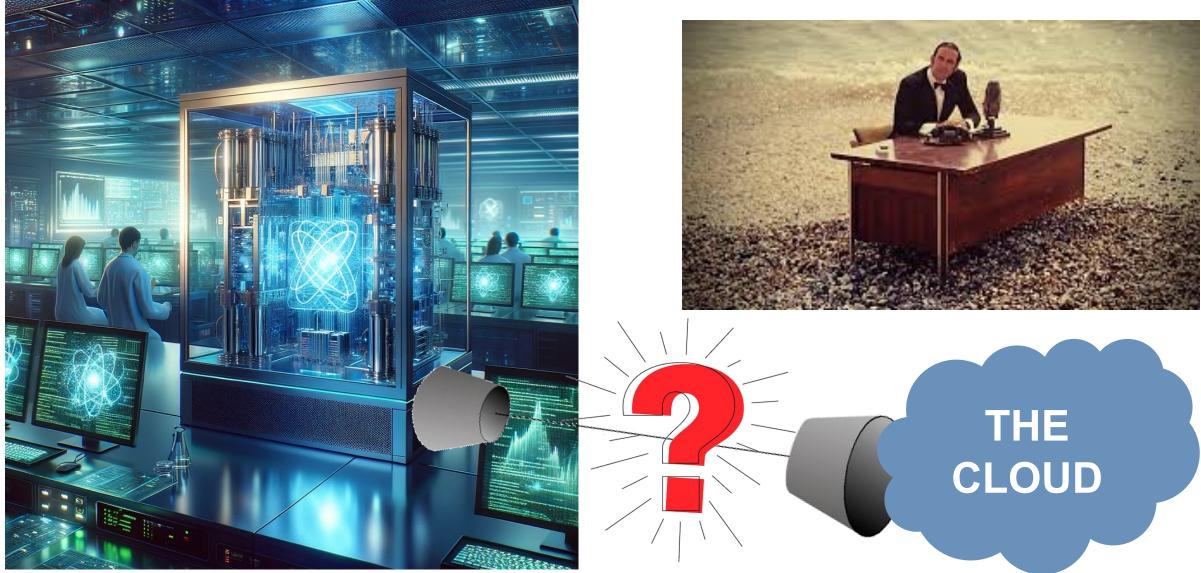
And Now to Something Completely Different!





And Now to Something Completely Different! Lot's of Excitement Around Quantum Computing









Quantum Computing: It is a Software Challenge, too! Martin Schulz @ APART 25th Anniversary Workshop Obergurgl, February 14th, 2024

What is all the Fuzz About? 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

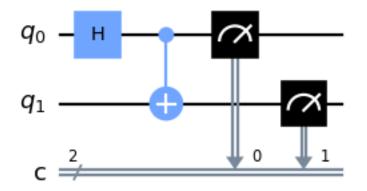
- Can be in superposed and/or entangled state
- When read: 0 or 1 only (rest collapses)

Programming with gates

- Operations on qubits
- Different systems have different gates

Quantum Advantage

 Some quantum algorithms require exponentially less steps than classical algorithms Martin Schulz @ APART 25th Anniversary Workshop, Obergurgl, February 14th, 2024



From: <u>https://docs.quantum.ibm.com/api/</u> giskit/giskit.circuit.QuantumCircuit



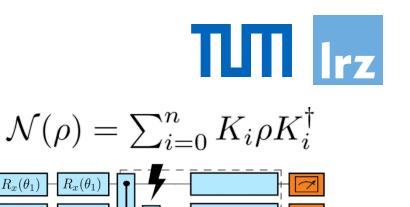
What is all the Fuzz About? Applications for Quantum Computing

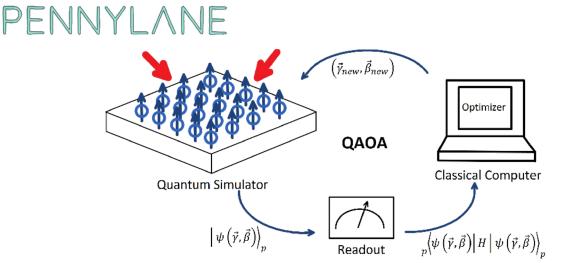
Main Application Domains

- Quantum simulation of quantum systems
- Quantum optimization
- Quantum machine learning
- Quantum linear systems

Problems:

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





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

Superconducting. Ion. Neutral Atom. Quantum-HPC.















Mission of MQV

Architect, Design, Implement and Deploy Full Stack Quantum Computing Systems In and for Bavaria

















Mission of Q-DESSI

Develop the Central Open Source Software Stack for Full Stack Quantum Computing Systems In and for Bavaria

For the MQV project For and co-funded by DAQC, Q-Exa, QuaST, MUNIQC-ATOMS/SC, ... For the for QC community















Mission and Goals of Q-DESSI

Q-DESSI provides programming & runtime env.

Compilers, Optimizers and Tools Secure multi-user environments Internal and external resource management

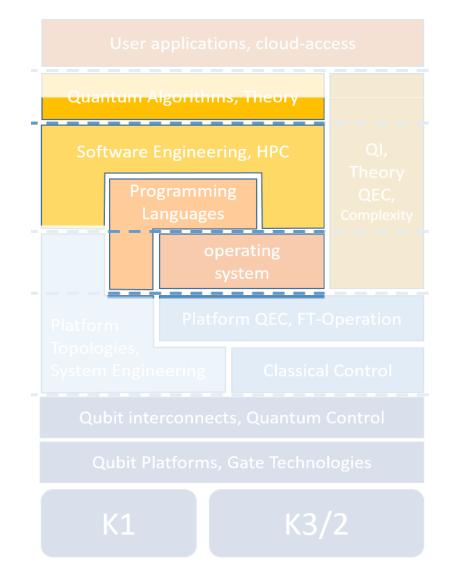
Q-DESSI provides integration with existing systems

Host platforms for control and analysis QC as accelerator for HPC Onloading of optimization/error correction to HPC

Four Focus Areas (aka. Central Tasks)

Programming Environments, Compilers and Tools Quantum OS and Runtime Quantum Control Microarchitecture & Firmware Integration with HPC & Cloud Systems





Quantum Computing So, Where Do We Stand?



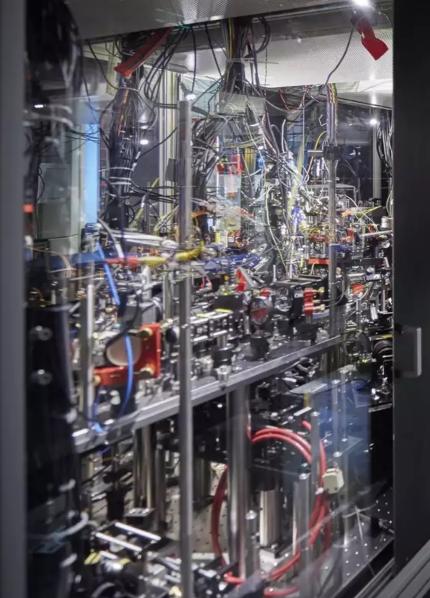


How will they look like? Artistics Renderings of Quantum Computers





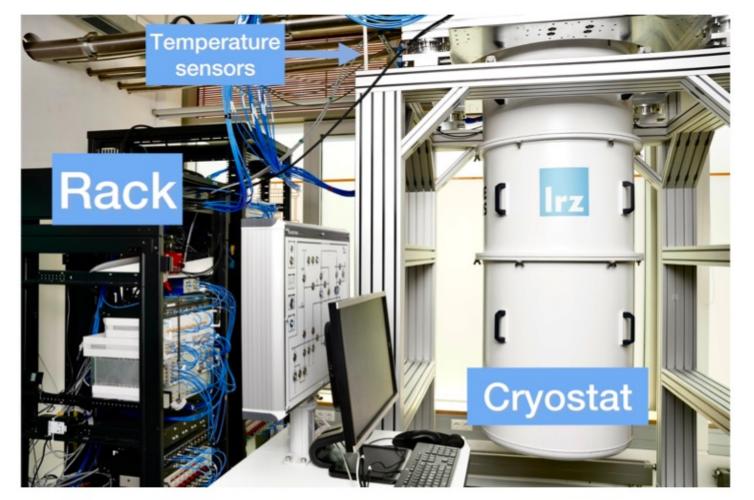
Quantum Computing as a Laboratory Experiment





First "Commercial" Systems at a Compute Center Examples in the LRZ Quantum Integration Centre (QIC)



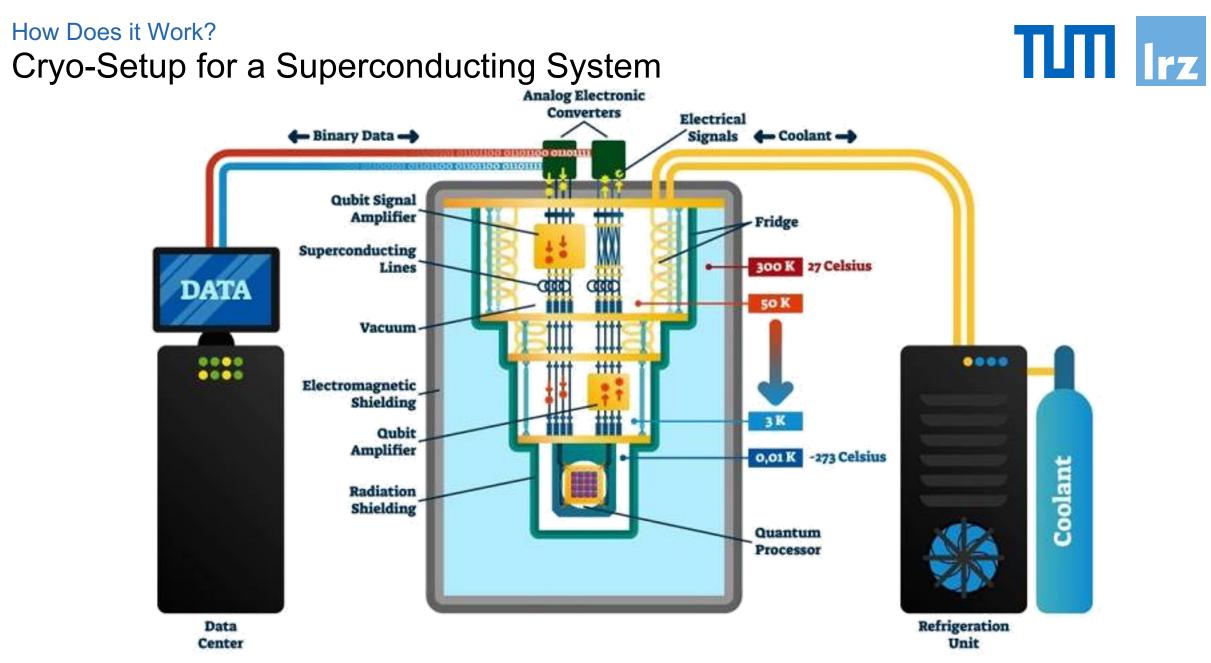


IQM @ LRZ

Martin Schulz @ APART 25th Anniversary Workshop, Obergurgl, February 14th, 2024



AQT @ LRZ

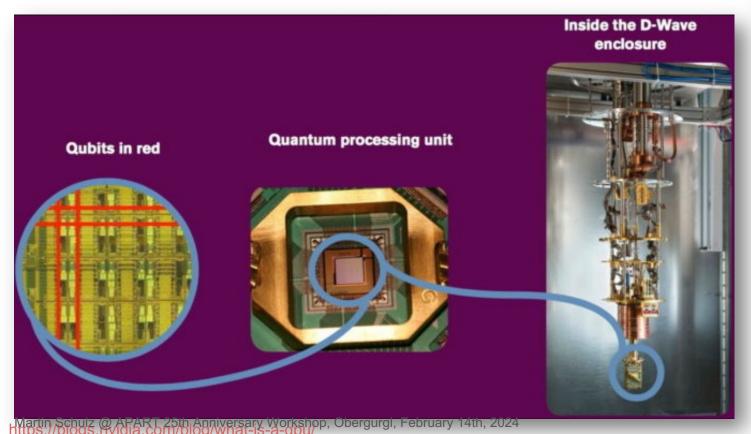


https://www.thebroadcastbridge.com/content/entry/14159/instant-answers-from-the-universe

How does it work?

The Quantum Processing Unit

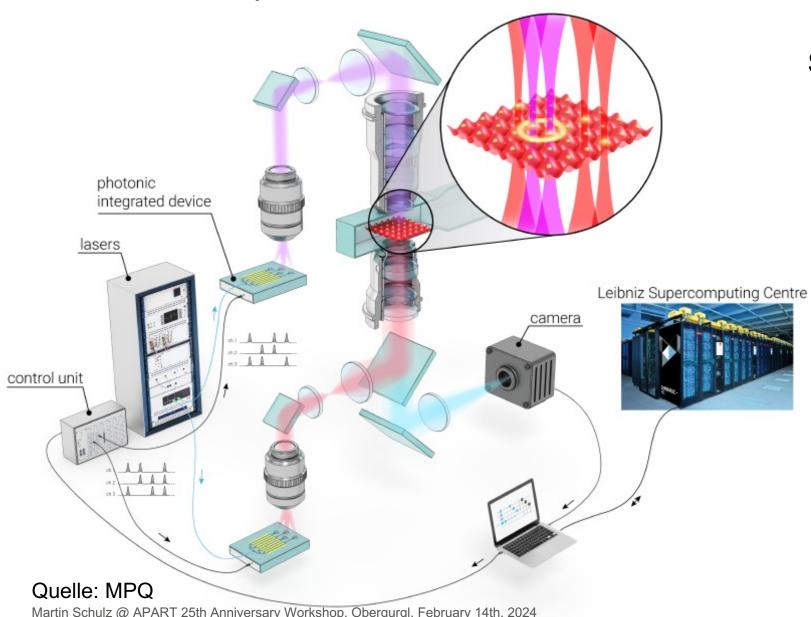
- Qubits are manufactured onto a chip
- Directly controlled from the outside
 - No internal control architecture
- Noisy intermediate scale quantum (NISQ)







How does it work? Second Example: Neutral Atoms



TIII lrz

Similar Structure

- Different Control
 - Laser instead of Microwave
- Different Qubits
 - Individual Atoms
- Again: separate external control system
- Again: classic compute to control the system







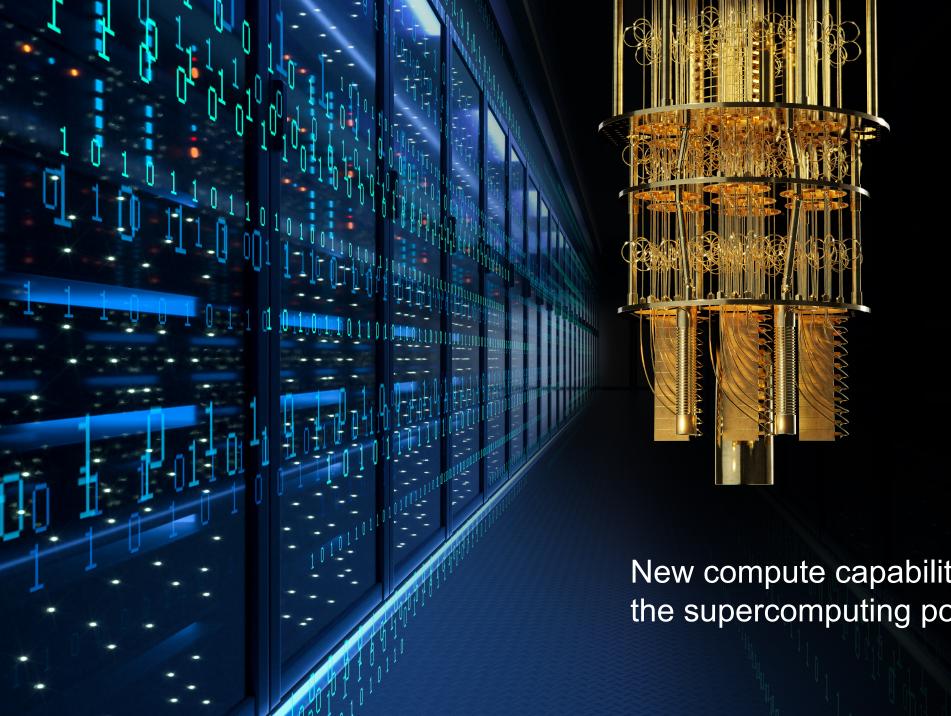
Quantum computers will not replace HPC.





Quantum computers will not replace HPC.

Quantum accelerators are HPC.



Why HPC-QC?

Quantum Computing High-Performance Computing

New compute capability that adds to the supercomputing portfolio.

HPCQC Integration Strategy: Quantum Computing as Accelerator for HPC



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

Usage exclusively as accelerator for HPC workloads

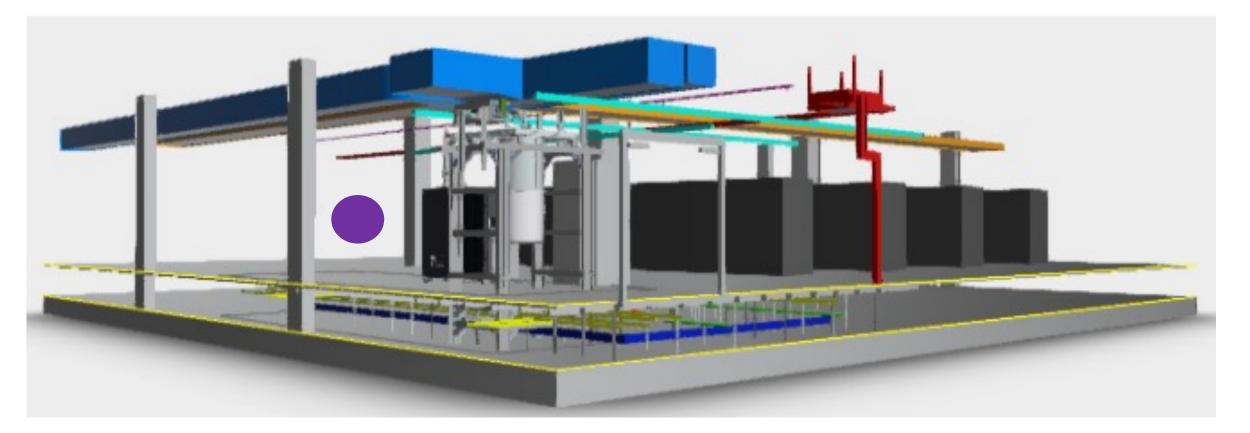
- Intended for fine-grained kernels within larger applications or workloads
- Similar to other accelerators, on-node (like GPUs, FPGAs) or dissaggregated (like AI HW)

Consequences: HPC and QC as a single HPCQC system

- Requires tools and models to extract application components relevant for acceleration
- Requires easy access for HPC community to QC programming (or library usage)
- Requires integration into a single programming environment
- Requires close hardware integration (single system) for latencies and management
- Requires unified user access/management/experience

LRZ QC and HPCQC Integration 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

System 2: ca. 20 qubits Vendor: IQM Accessible: H1-2024 to select research partners

System 3: 20 qubits

Vendor: IQM Accessible: Late H1-2024 to Bavarian, German and European users in pilot phase initially, wider access in 2024

System 4: 50+ qubits

Vendor: TBD Accessible: Early H2-2025 to Bavarian, German and European users

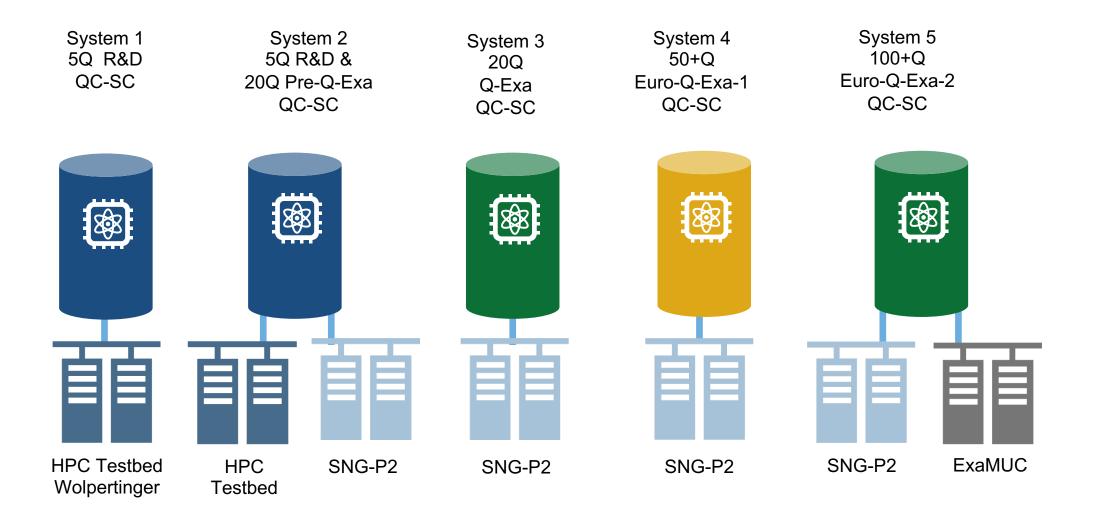
System 5: 100+ qubits

Vendor: TBD Accessible: Early H1-2026 to Bavarian, German and European users



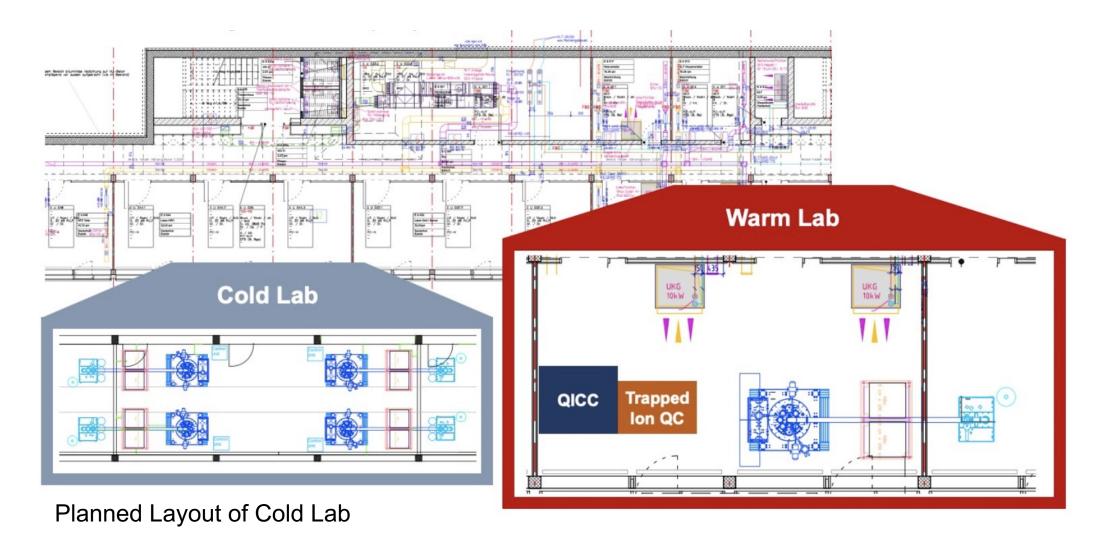
LRZ Quantum Systems Superconducting Systems Roadmap with HPC





Lab Setup Quantum Integration Centre (QIC)





Lab Setup Quantum Integration Centre (QIC)



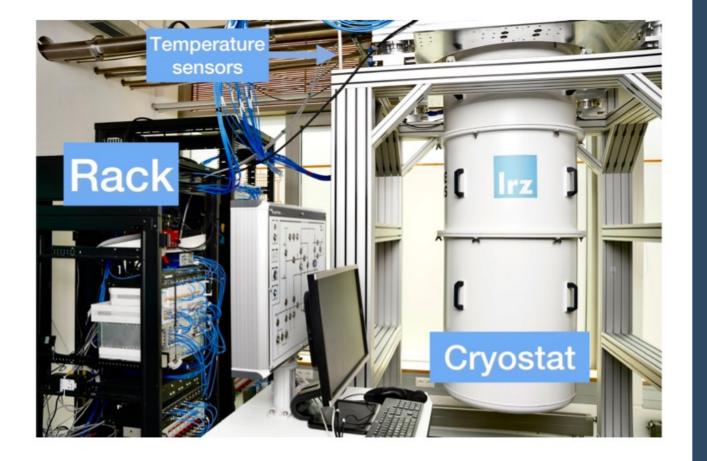


Martin Schulz @ APART 25th Anniversary Workshop, Obergurgl, February 14th, 2024

Source: MPQ

Challenges in Integration Integration into HPC Center Telemetry





HPC Center Monitoring

System and Infrastructure Health Application Performance

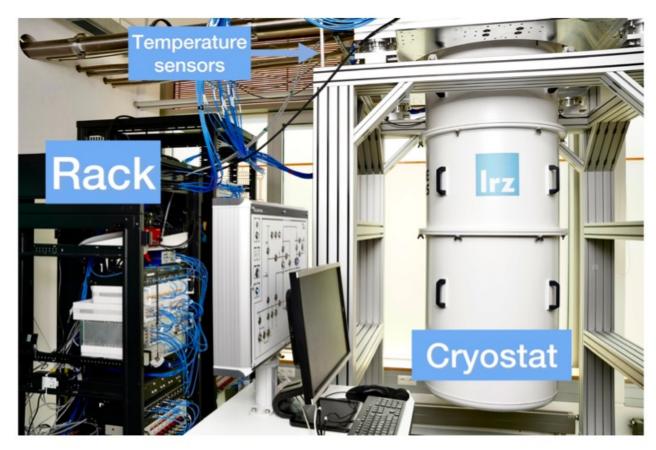
Inclusion of QC

From Cryostat to Control Electronics IoT Infrastructure needed Plus: Key metrics like fidelity

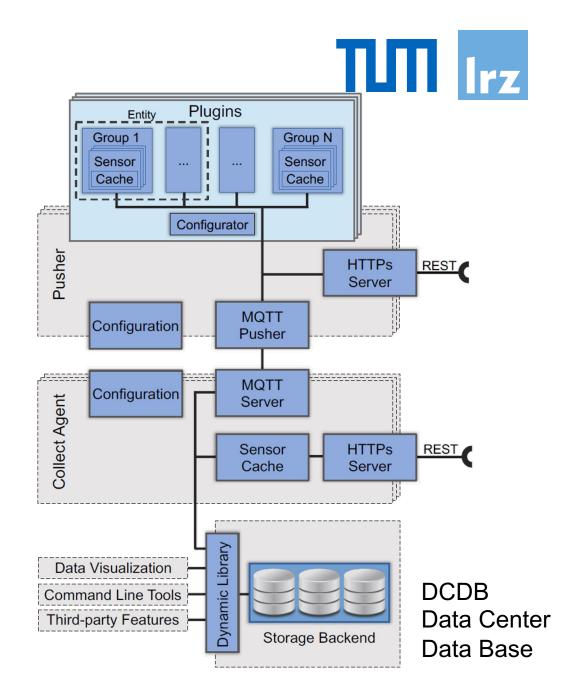
Operational Data Analytics

Towards predictive / hands-off maintenance

Challenges in Integration Integration into HPC Center Telemetry



For more on this: talk by Hossam Anmed at the WIHPQC23 workshop today



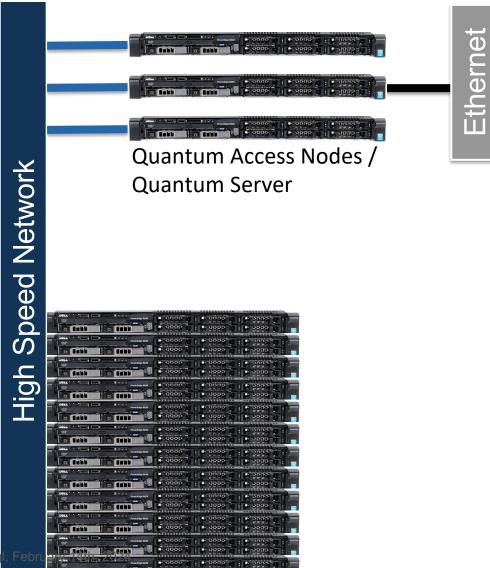
How does work in Hardware? Integration von QC und HPC

Connection to the HPC network

Direct connection to QC controller

BUT: It has to be a full stack solution!

Martin Schulz @ APART 25th Anniversary Workshop, Obergurg











Infrastructure	Standalone system with own monitoring	Integrated in data center with cooling, power/energy, monitoring
Hardware	Quantum Computing Appliance + HPC System	Single system with integrated QC accelerator(s)
Software	Two separate software stacks with "glue scripts"	Single-source programming with high-level abstractions
Applications	Algorithms with quadratic speedup and separate QC and HPC applications	Algos with faster speedup and truly hybrid applications
Culture	Computer Science, Math, Electrical Engineering, Physics communities	Hybrid HPCQC community

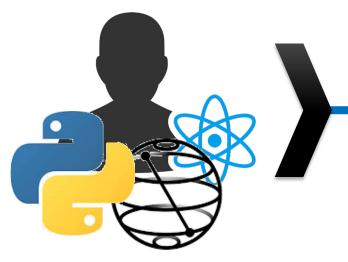


Some HPCQC End Goals

Infrastructure	Standalone system with own monitoring	Integrated in data center with cooling, power/energy, monitoring
Hardware	Quantum Computing Appliance + HPC System	Single system with integrated QC accelerator(s)
Software	Two separate software stacks with "glue scripts"	Single-source programming with high-level abstractions
Applications	Algorithms with quadratic speedup and separate QC and HPC applications	Algos with faster speedup and truly hybrid applications
Culture	Computer Science, Math, Electrical Engineering, Physics communities	Hybrid HPCQC community

Supporting the Needed Transition the Laboratory to Production Current State of Software

Individual Physics Researcher



Quantum Device





Supporting the Needed Transition the Laboratory to Production Challenges in Current Software Setup

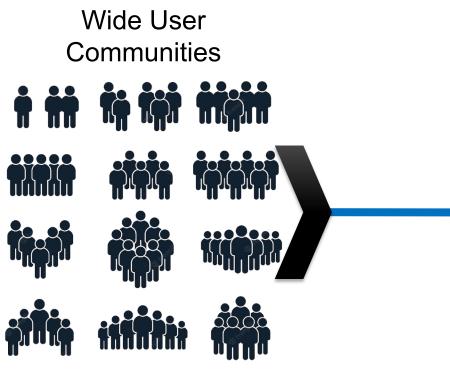


Individual Quantum **Physics** Device Researcher



Supporting the Needed Transition the Laboratory to Production Requirements





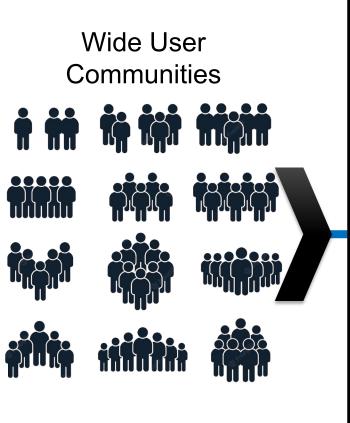




Many/Different Quantum Devices

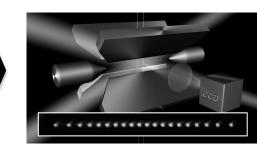
Supporting the Needed Transition the Laboratory to Production Requirements





Comprehensive Software Stack

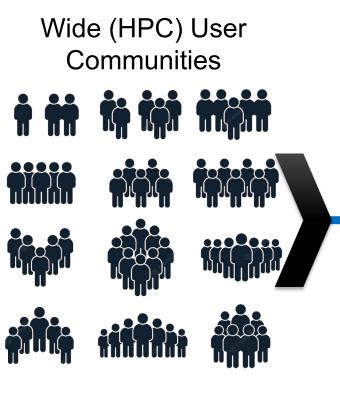






Many/Different Quantum Devices Supporting the Needed Transition the Laboratory to Production Requirements

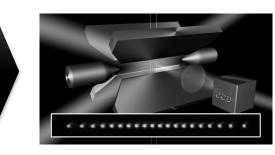




Comprehensive Software Stack

integrated into HPC Environments



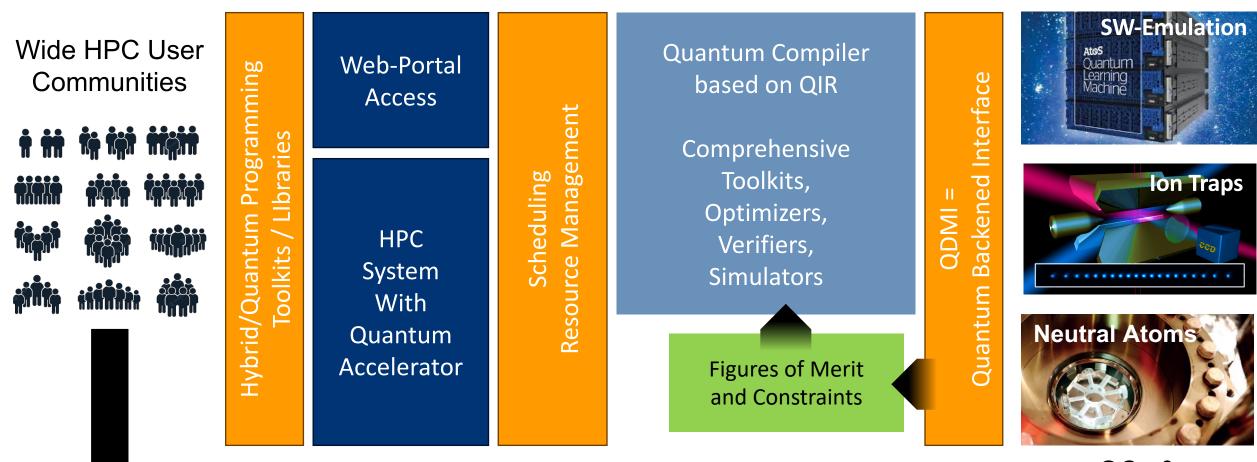




Many/Different Quantum Devices

The Munich Quantum Software Stack (MQSS) MQSS Overview





Enabling Domain User Communities to Compute on Quantum Devices

QCs & Simulators

The Munich Quantum Software Stack (MQSS) Front-End / Languages





Different Programming Models

- Standard approaches like Qiskit/Pennylane
- Higher-level abstractions
 - Incl. those provided by QLM
- New developments
- HPCQC approaches, like OpenMP
- Domain specific support

Decoupled from compilation stack

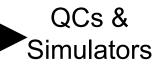
- Multiple front-ends, one backend
- Translation into standard format
 - QIR establishing itself as standard
- Result: Templated circuits

Enabling Domain User Communities to Compute on Quantum Devices









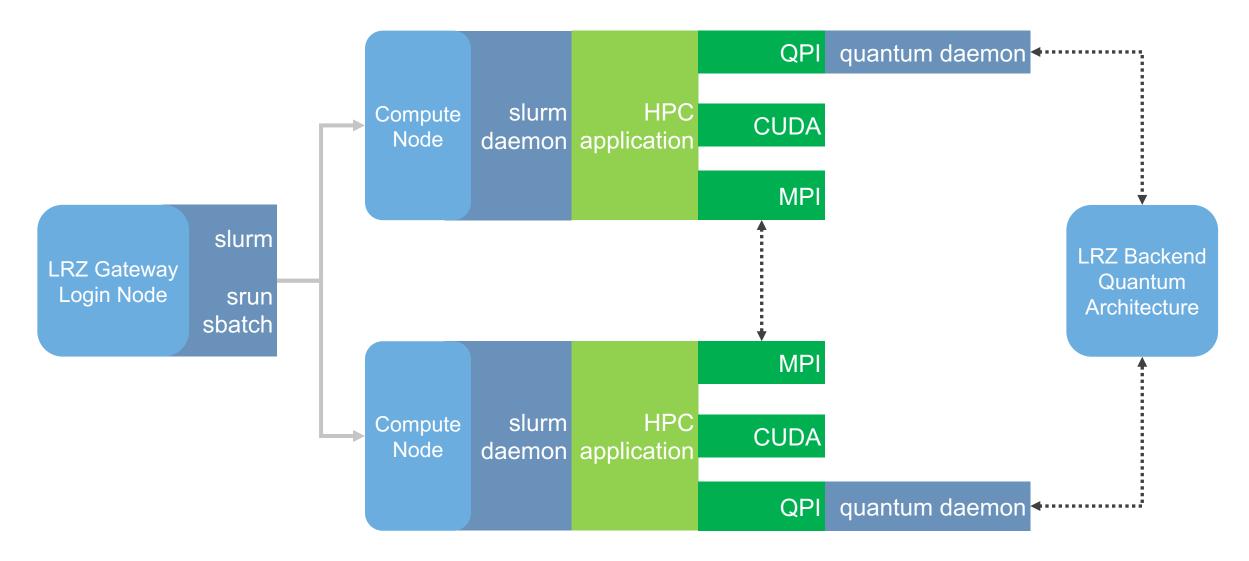
QC and HPCQC System Software Quantum Programming Interface

- 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

1	#define QPI_1
2	<pre>#include <qpi.h> #include <stdio.h></stdio.h></qpi.h></pre>
3	<pre>#include <stdio.h></stdio.h></pre>
4	
5	
6	<pre>void bell_0() {</pre>
7	Qcircuit circuit;
8	Qstatus status;
9	
0	<pre>int states = 4;</pre>
1	int shots = 1000;
2	
.3	<pre>// 4 states can exist with 2 qubits</pre>
4	<pre>int output[states];</pre>
.5	
.6	<pre>qCircuitBegin(&circuit);</pre>
.7	
.8	qH(0);
9	qCX(0, 1);
20	
21	<pre>qMeasure_all();</pre>
22	
23	<pre>qCircuitEnd();</pre>
24	
25	<pre>qExecute(circuit, shots, &status);</pre>
26	<pre>qWait(status);</pre>
27	
28	<pre>qRead(status, QPI_READ_ALL_STATES, (int*)&output);</pre>
29	
30	<pre>for(int state_idx=0; state_idx < states; state_idx++) {</pre>
31	<pre>printf(" %d>: %d", state_idx, output[state_idx]);</pre>
32	}
33	}

QC and HPCQC System Software HPC Accessing QC via QPI

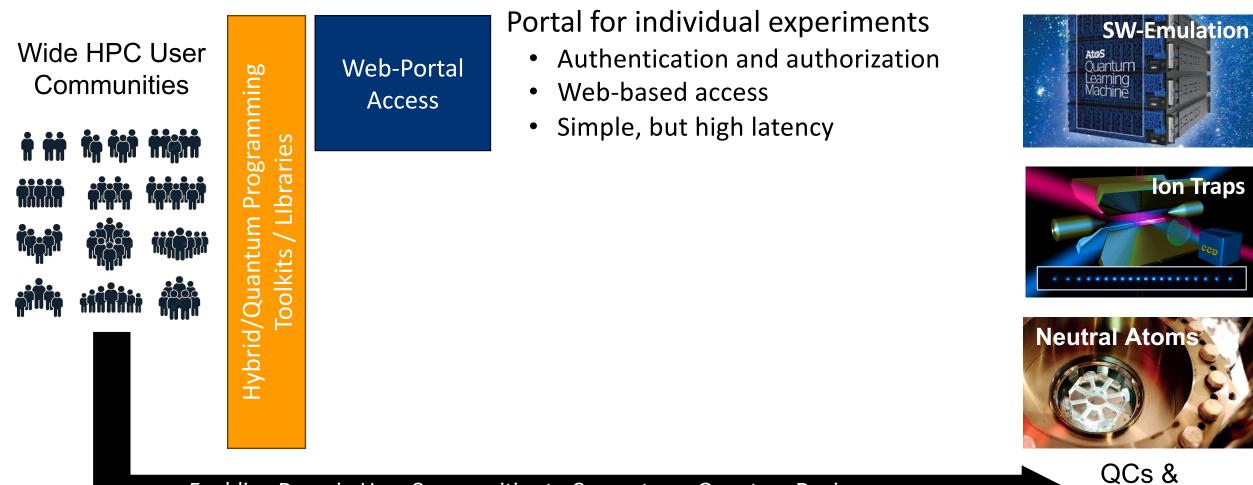




The Munich Quantum Software Stack (MQSS) Portal Access (aka. "Cloud Access")



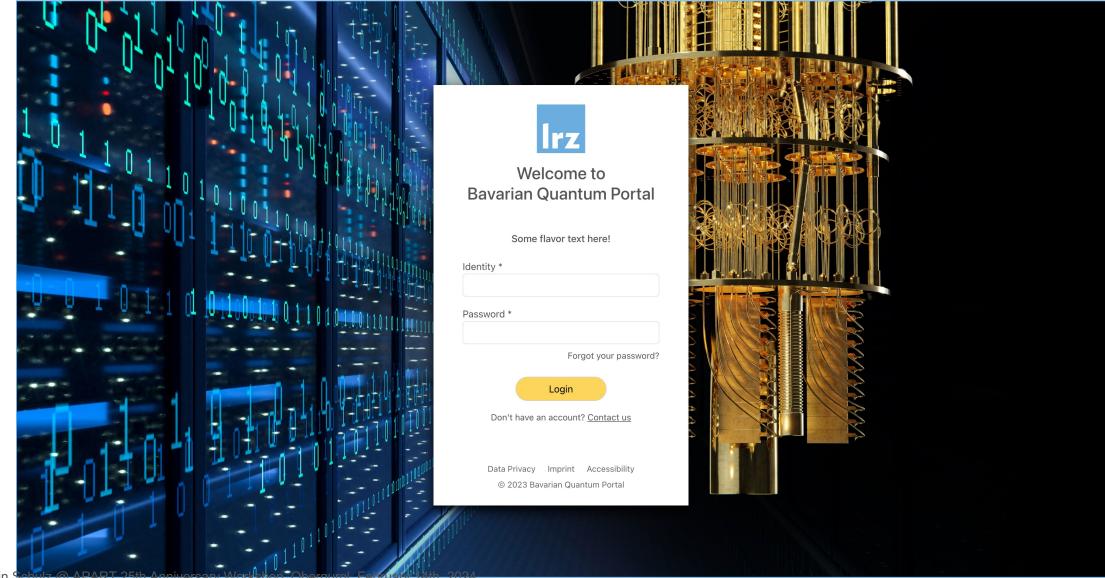
Simulators



Enabling Domain User Communities to Compute on Quantum Devices

The Munich Quantum Software Stack (MQSS) The Bavarian Quantum Portal (BQP)



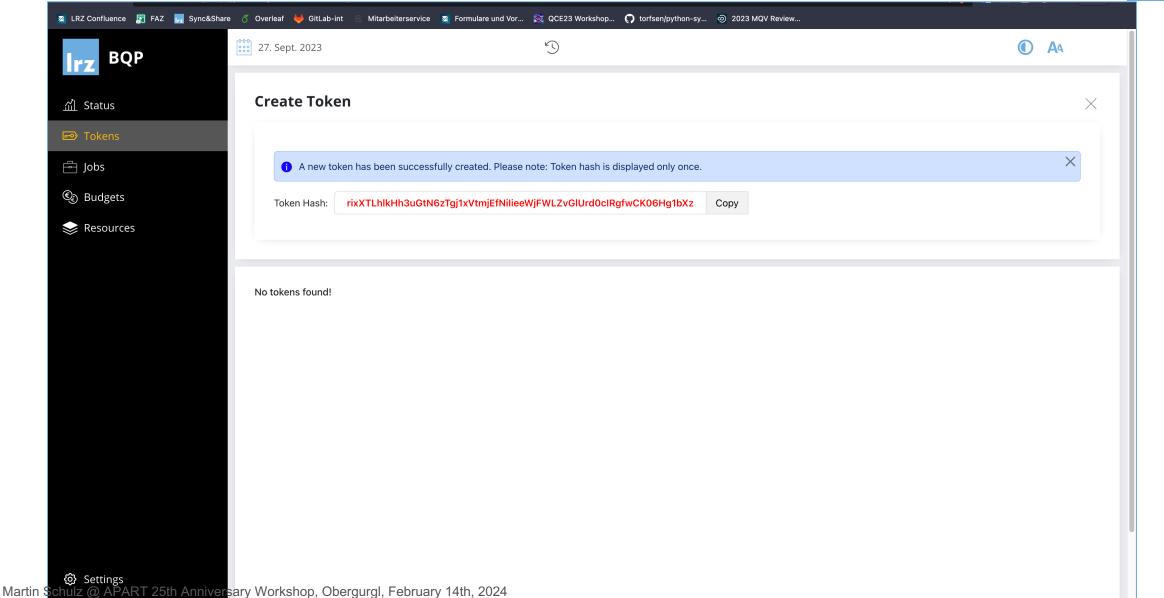


The Munich Quantum Software Stack (MQSS) BQP Sample Usage

Martin

BQP 27. Sept. 2023	Ś		Aq
S Create Token			>
INS (*) Required field			
Token Name *		Maximum Job Count *	
ets Demo1		•	30/100
Validity *		Maximum Budget Usage *	
	● 4/7 day(s)	•	23083/100000
Valid From *			
27.09.2023			
Expiration (read only)			
Submit Cancel			
No tokens found!			

The Munich Quantum Software Stack (MQSS) BQP Sample Usage (cont.)



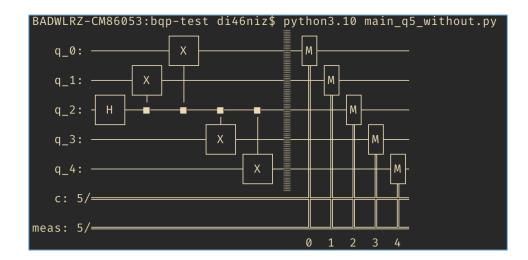
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The Munich Quantum Software Stack (MQSS) BQP Qiskit Provider

	from bavarian_quantum_portal_provider import BQPProvider
	from pprint import pprint
7 8	import termplotlib as tpl
	ifname == "main":
11	c = QuantumCircuit(5, 5)
	c.h (2)
16	
18	
19 20	
20	
22	
	<pre>provider = BQPProvider(token=tokenfile.read()[:-1])</pre>
26	backend = provider.get_backend("Test Q5")
28	
30 31	
32	
33	
34	
35	
	}
38	
40	
42 43	force_ascii=False,
	; fig.show()
44	115.510W()
46	



The Munich Quantum Software Stack (MQSS) BQP Python Execution

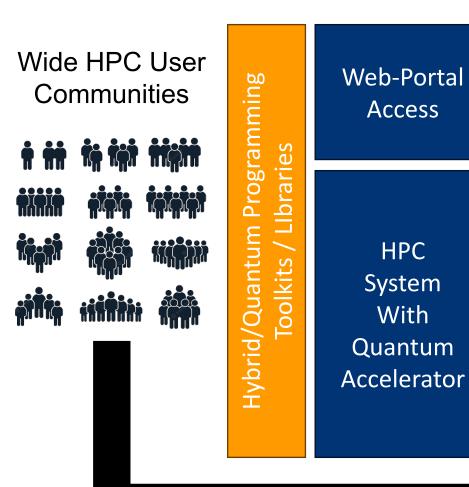


ПП '00000': 309, '00001': 58, '00010': 78, '00011': 16, '00101': 7, '00110': 1, '00111': 3, '01000': 26, '01001': 5, '01010': 5, '01011': 1, '01100': 2, '01101': 10, '01110': 2, '01111': 19, '10000': 15, '10001': 6, '10010': 4, '10011': 2, '10100': 8, '10101': 19, '10110': 2, '10111': 33, '11000': 3, '11001': 6, '11011': 2, '11100': 22, '11101': 128, '11110': 34, '11111': 174} .RZ-CM86053:bap-test di46niz\$ BADWI

Irz

The Munich Quantum Software Stack (MQSS) HPC Access





Portal for individual experiments

- Authentication and authorization
- Web-based access
- Simple, but high latency

Access via HPC System

- Submission to HPC scheduler as regular HPC job
- Access to QC system from HPC job
- Offload / Host-based interfaces
 - E.g., OpenMP target

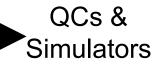
In both cases: result is a templated circuit to be executed

Enabling Domain User Communities to Compute on Quantum Devices

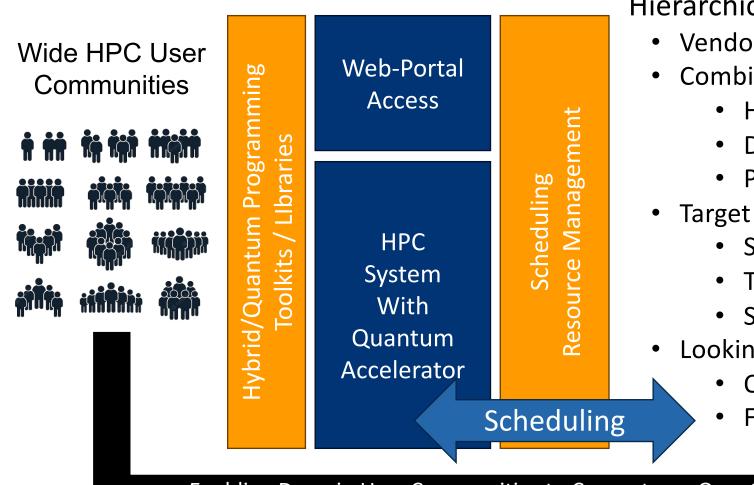








The Munich Quantum Software Stack (MQSS) Scheduling & Resource Management



Hierarchical Scheduling Component

- Vendor neutral, open source
- Combining/Coordinating
 - HPC Scheduler (given by center)
 - Device Scheduler (intermediary)
 - Platform Scheduler (given by vendor)

QC &

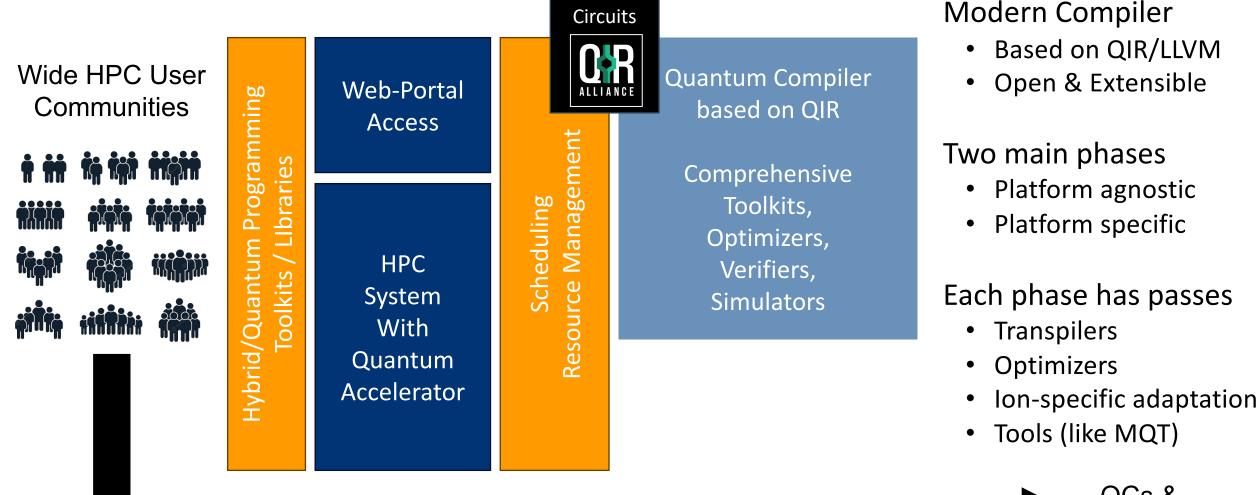
Simulators

- Target platform selection
 - Simulator vs. Hardware Device
 - Type of modality
 - Suitable device within modality
- Looking at new scheduler technologies
 - OAR (Grenoble)
 - Flux (LLNL)

Enabling Domain User Communities to Compute on Quantum Devices

The Munich Quantum Software Stack (MQSS) Quantum Compiler



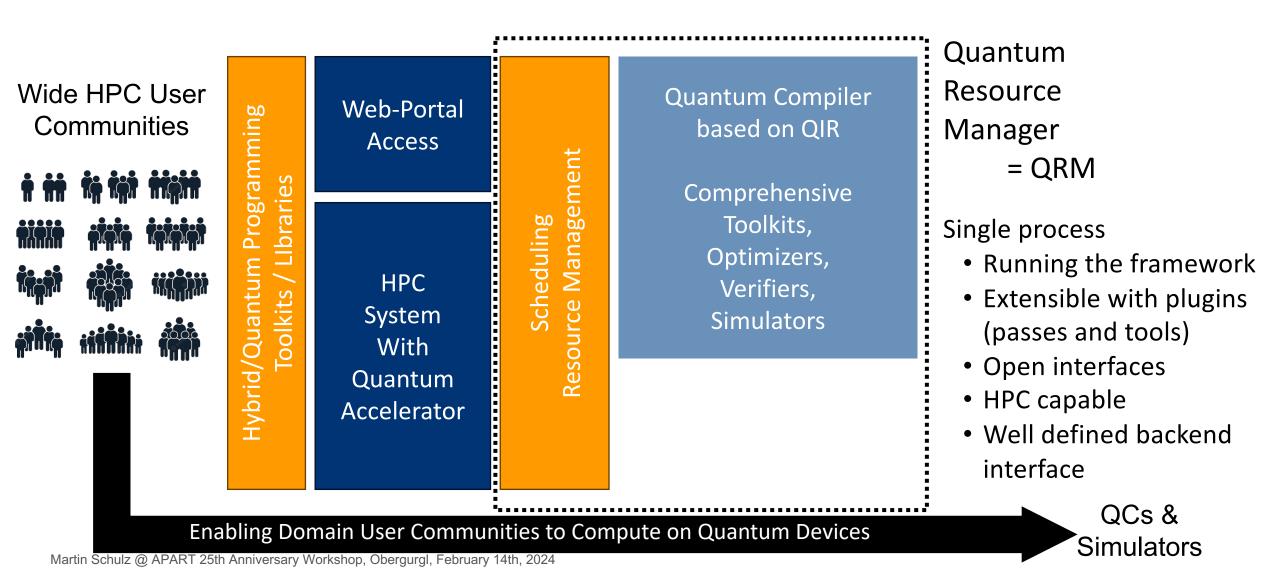


Enabling Domain User Communities to Compute on Quantum Devices

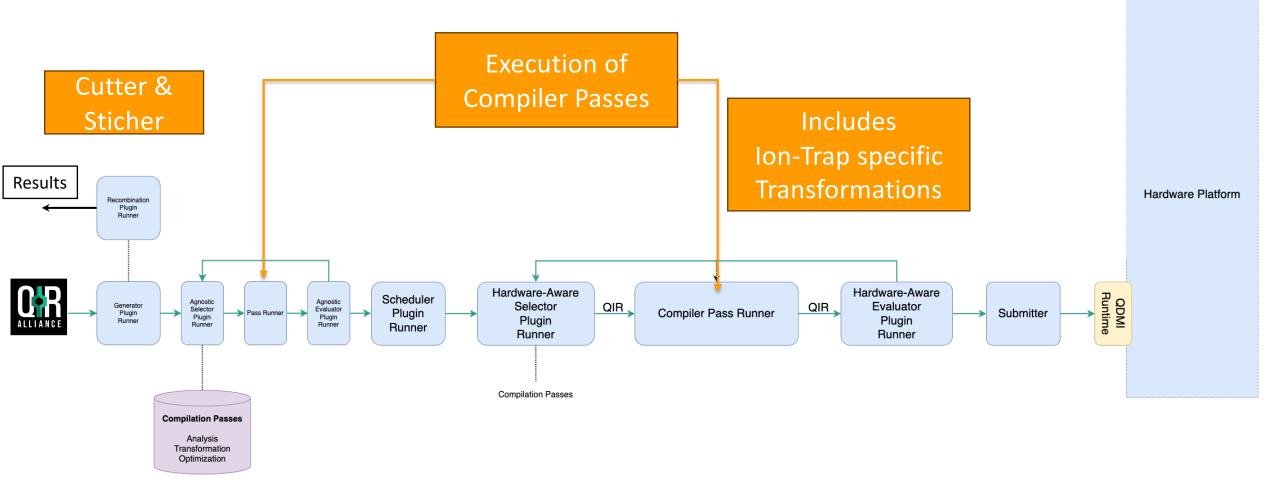
QCs & Simulators

The Munich Quantum Software Stack (MQSS) Quantum Resource Manage





Compilation Process in the MQSS Driving an LLVM-based open compilation infrastructure



Platform agnostic

Platform specific

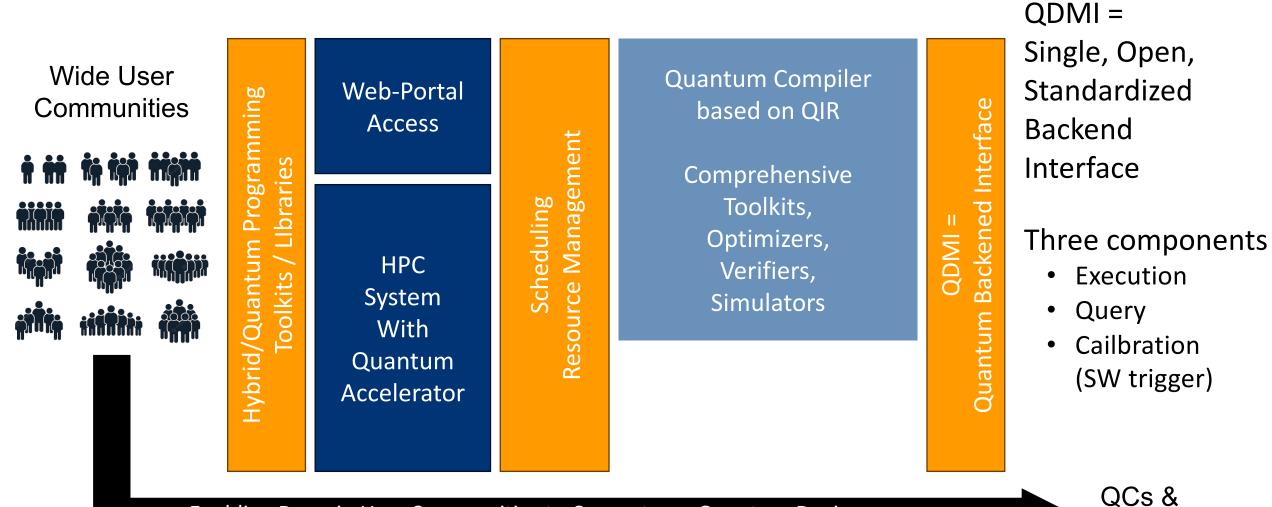
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The Munich Quantum Software Stack (MQSS) The QDMI Backend



Simulators



Enabling Domain User Communities to Compute on Quantum Devices

The Munich Quantum Software Stack (MQSS) QDMI Basics



C-API to access QC systems from compilation backend (QDMI Control)

- API is Platform neutral
- Core implementation maps API to a backend plugin

The Munich Quantum Software Stack (MQSS) QDMI Core



Find and Instantiate Devices

/* Core Session, basic start/close routines */

int QDMI_session_init(QInfo info, QDMI_Session *session); int QDMI_session_finalize(QDMI_Session session);

/* Core Interface */

The Munich Quantum Software Stack (MQSS) QDMI Basics



C-API to access QC systems from compilation backend (QDMI Control)

- API is Platform neutral
- Core implementation maps API to a backend plugin
- System specific backends
- Remote forwarding option for systems not located at LRZ (higher latency, loose coupling, but access and execution possible)

The Munich Quantum Software Stack (MQSS) QDMI Control



Create, Submit and Control QC jobs, Read Results

int QDMI control pack gasm2(QDMI Device dev, char *gasmstr, QDMI Fragment *frag); int QDMI control pack gir(QDMI Device dev, void *girmod, QDMI Fragment *frag); int QDMI_control_submit(QDMI_Device dev, QDMI_Fragment *frag, int numshots, QInfo int QDMI control cancel(QDMI Device dev, QDMI Job *job, QInfo info); int QDMI_control_pause(QDMI_Device dev, QDMI_Job *job, QInfo info); int QDMI control test(QDMI Device dev, QDMI Job *job, int *flag, QDMI Status *status); int QDMI_control_wait(QDMI_Device dev, QDMI_Job *job, QDMI_Status *status); int QDMI control extract state(QDMI Device dev, QDMI Status status, int *state); int QDMI control readout size(QDMI Device dev, QDMI Status *status, int *numbits); int QDMI control readout hist size(QDMI Device dev, QDMI Status *status, int *size); int QDMI control readout hist top(QDMI Device dev, QDMI Status *status, int numhist, QInfo info, long *hist); int QDMI control readout raw num(QDMI Device dev, QDMI Status *status, int *num); int QDMI control_readout_raw_sample(QDMI_Device dev, QDMI_Status *status, int numraw, QInfo

info, long *hist);

The Munich Quantum Software Stack (MQSS) QDMI Basics



C-API to access QC systems from compilation backend (QDMI Control)

- API is Platform neutral
- Core implementation maps API to a backend plugin
- System specific backends
- Remote forwarding option for systems not located at LRZ (higher latency, loose coupling, but access and execution possible)

API for functionality to read dynamic data from QC system (QDMI Query)

- Enable proper selection of suitable backends
- Usage by compilation passes to drive optimizations

The Munich Quantum Software Stack (MQSS) QDMI Query



Ask for system properties, gate sets and gate properties (e.g., fidelities)

int QDMI_query_device_property_exists(QDMI_Device dev, QDMI_Device_property prop, int* scope); int QDMI_query_device_property_i(QDMI_Device dev, QDMI_Device_property prop, int *value); int QDMI_query_device_property_f(QDMI_Device dev, QDMI_Device_property prop, float *value); int QDMI_query_device_property_d(QDMI_Device dev, QDMI_Device_property prop, double *value);

int QDMI_query_gateset_num(QDMI_Device dev, int *num_gates); int QDMI_query_one_gate(QDMI_Device dev, QDMI_Gate *gate); int QDMI_query_all_gates(QDMI_Device dev, QDMI_Gate *gates); int QDMI_query_byname(QDMI_Device dev, char *name, QDMI_Gate *gate);

int QDMI_query_gate_name(QDMI_Device dev, QDMI_Gate gate, char* name, int* len);
int QDMI_query_gate_size(QDMI_Device dev, QDMI_Gate gate, int* gatesize);
int QDMI_query_gate_unitary(QDMI_Device dev, QDMI_Gate gate, QDMI_Unitary *unitary);

The Munich Quantum Software Stack (MQSS) QDMI Basics



C-API to access QC systems from compilation backend (QDMI Control)

- API is Platform neutral
- Core implementation maps API to a backend plugin
- System specific backends
- Remote forwarding option for systems not located at LRZ (higher latency, loose coupling, but access and execution possible)

API for functionality to read dynamic data from QC system (QDMI Query)

- Enable proper selection of suitable backends
- Usage by compilation passes to drive optimizations

API to Access to regular re-calibration (QDMI Device)

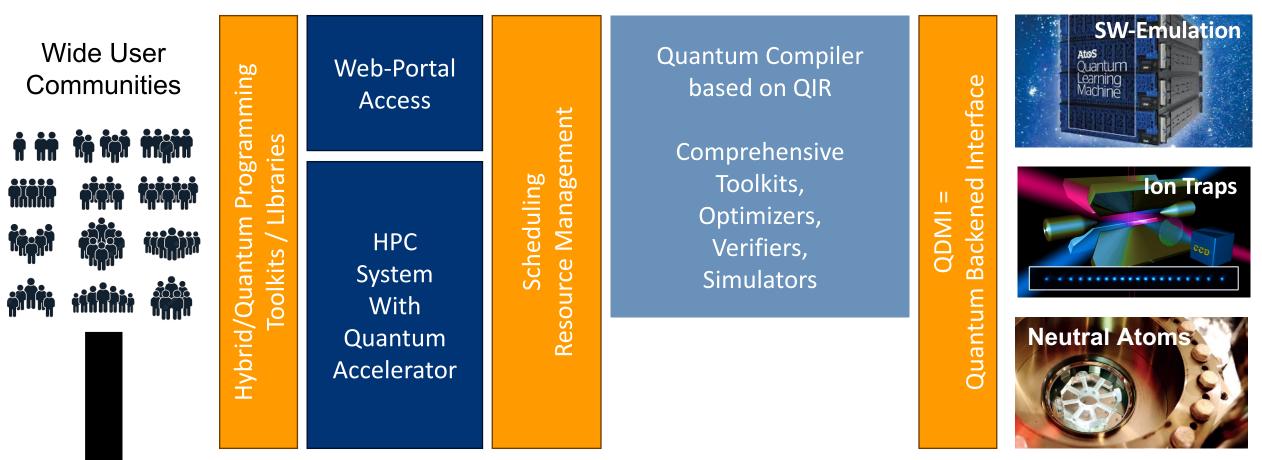
The Munich Quantum Software Stack (MQSS) QDMI Device

Access to re-calibration

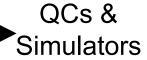
int QDMI_device_status(QDMI_Device dev, QInfo info, int *status); int QDMI_device_quality_check(QDMI_Device dev, double *result); int QDMI_device_quality_limit(QDMI_Device dev, double *result); int QDMI_device_quality_calibrate(QDMI_Device dev); IIII Irz

The Munich Quantum Software Stack (MQSS) End-to-End to the Systems



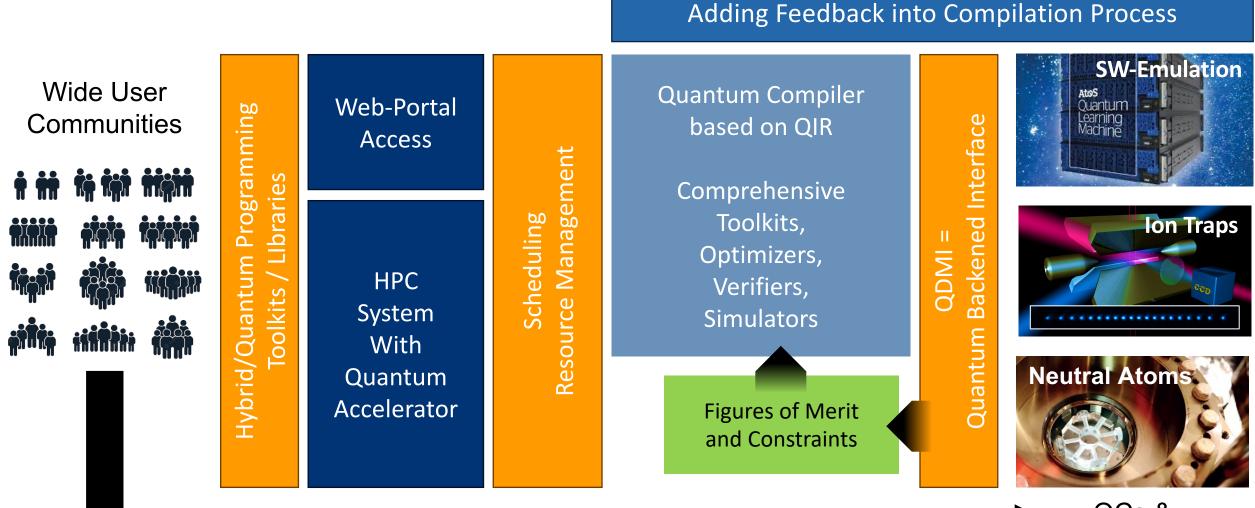


Enabling Domain User Communities to Compute on Quantum Devices



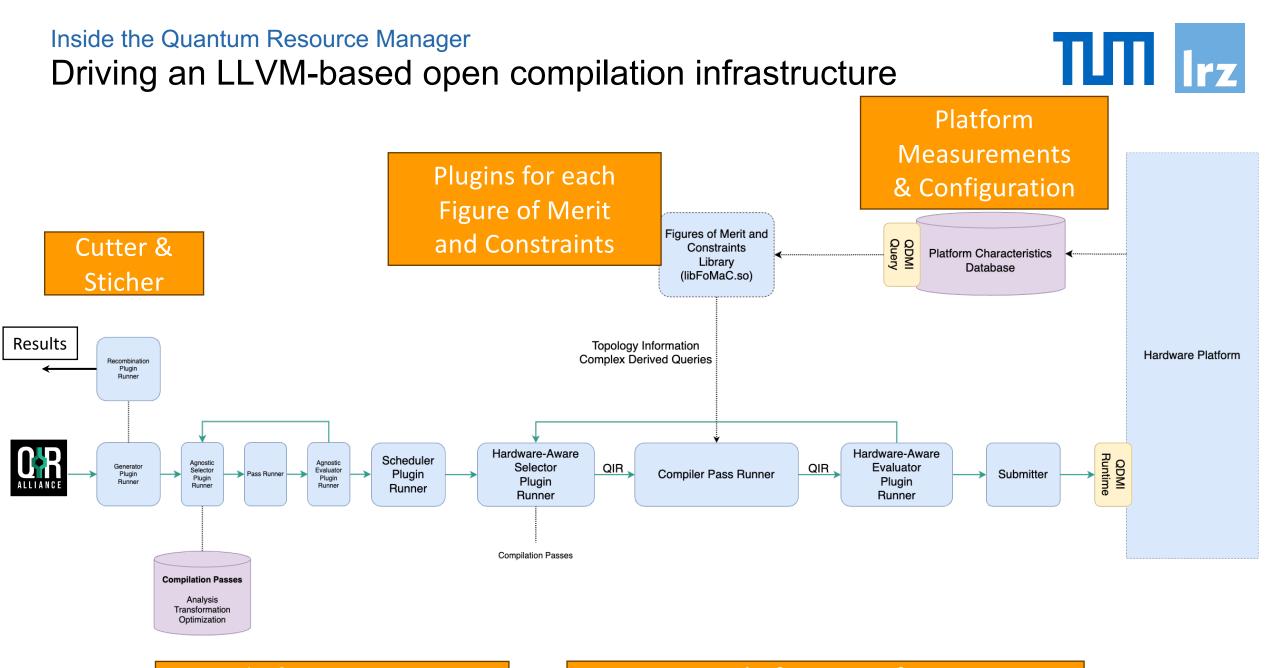
The Munich Quantum Software Stack (MQSS) Feedback from the Target System





Enabling Domain User Communities to Compute on Quantum Devices

QCs & Simulators



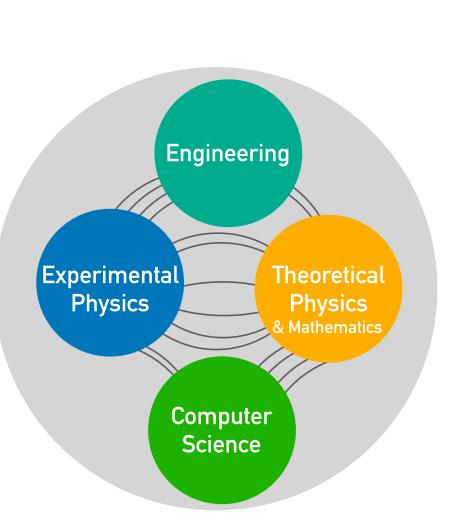
Platform agnostic

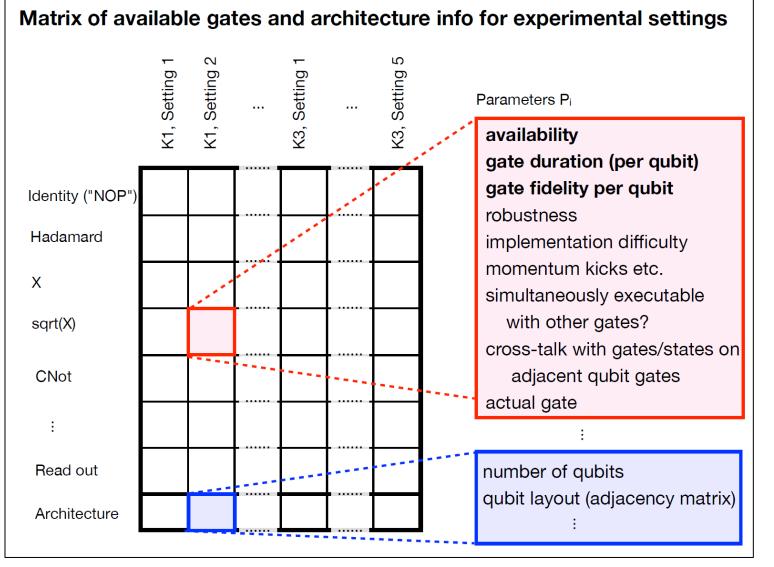
Martin Schulz @ APART 25th Anniversary Workshop, Obergurgl, February 14th, 2024

Platform specific

Feedback from Quantum System Representing Figures of Merit



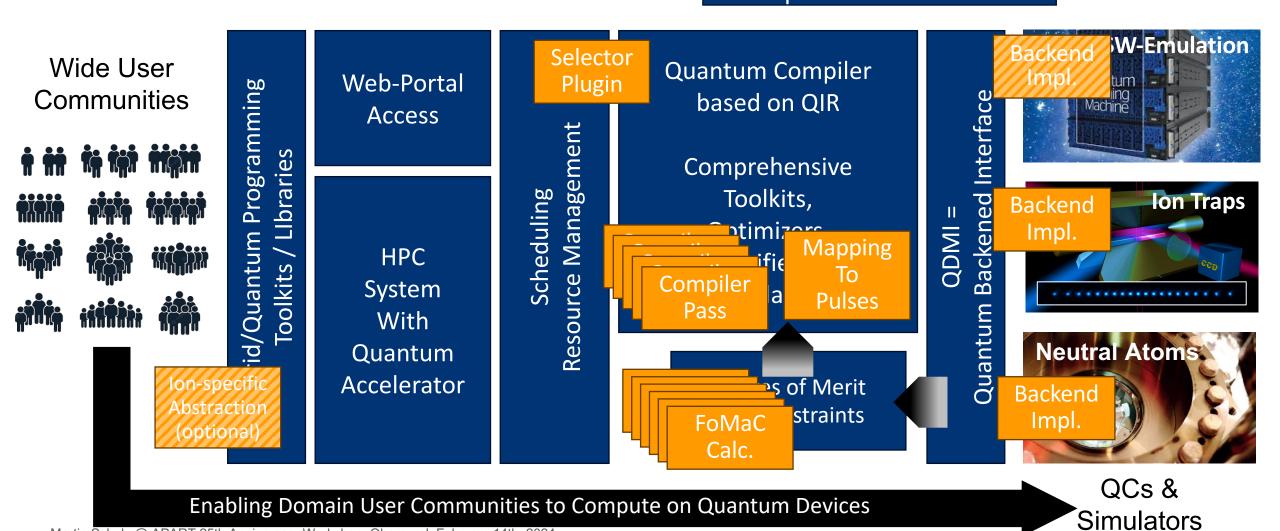




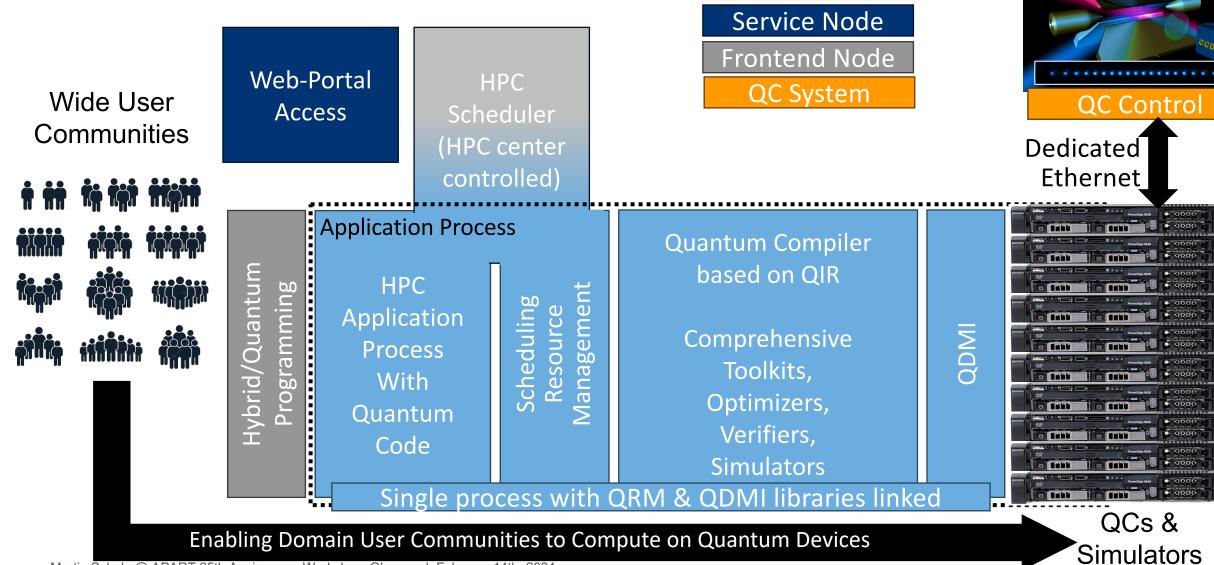
The Munich Quantum Software Stack (MQSS) Separating Concerns



Plattform Component **Open Infrastructure**



The Munich Quantum Software Stack (MQSS) Architecture Mapping to Hardware



Compute Node

on Traps



Some HPCQC End Goals

Infrastructure	Standalone system with own monitoring	Integrated in data center with cooling, power/energy, monitoring
Hardware	Quantum Computing Appliance + HPC System	Single system with integrated QC accelerator(s)
Software	Two separate software stacks with "glue scripts"	Single-source programming with high-level abstractions
Applications	Algorithms with quadratic speedup and separate QC and HPC applications	Algos with faster speedup and truly hybrid applications
Culture	Computer Science, Math, Electrical Engineering, Physics communities	Hybrid HPCQC community



European Quantum System Software Summit April 19-21, 2023 Raitenhaslach

vare Summit



European Quantum System Software Summit July 11-13, 2023 LRZ



Quantum-HPC Working Group

Building a global community for sustained, structured engagements

Developing community-driven best practices for deploying, operating and using hybrid HPC-QCS systems, tools and applications

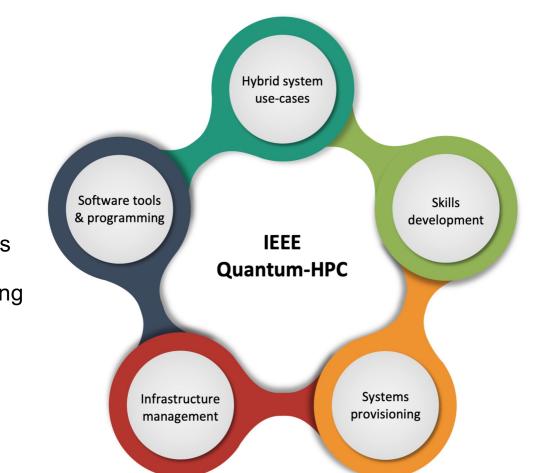
- Launched at IEEE QCE23 (September 2023)
- SC23 BOF Session (November 2023)
- More BoFs/Events/Workshops planned





Read more at quantum.ieee.org/working-groups

or grab the QR code



Towards Practical Quantum Computing It is a Software Challenge, too!



A Comprehensive Software Stack is Key for QC Systems

- Enables wide range of user communities
- Delivers efficient workflows from code to optimized pulses
- Provides safe production-level multi-user operations

QC must be integrated into existing HPC environments

- Targets specific computational problems
- Is part of larger hybrid workflows
- Relies on HPC resources for optimization
- 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!

CAPS Team @ TUM



From the MQV Review Meeting 2022

Martin Schulz @ APART 25th Anniversary Workshop, Obergurgi, February 14th, 2024



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and Research

Federal Ministry for Economic Affairs and Climate Action







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MQT

