QUANTUM COMPUTING AT THE DLR INSTITUTE OF SOFTWARE TECHNOLOGY - ALGORITHMS AND APPLICATIONS

Institute of Software Technology

Department High-Performance Computing

Dr.-Ing. Achim Basermann, Department Head *High-Performance Computing*

DLR

Survey

- DLR, Institute of Software Technology (SC) and
  its High-Performance Computing Department (SC-HPC)
- The DLR Quantum Computing Initiative
- Quantum Computing (QC) at SC-HPC: Big Picture
- QC at SC-HPC: Details
- Selected QC Applications at DLR
- Optional: DLR´s QC Solution Center in Hamburg

DLR

German Aerospace Center

Bild: Nonwarit/Fotolia

- Research Center
  - Research and development in aeronautics, space, energy, transportation, digitalization, as well as security and safety
  - National and international cooperations

- Space agency
  - Planing and realization of German space activities

- Funding agency
  - Research funding and project administration

DLR Locations and Employees

More than 10,000 employees across
55 institutes and facilities at
30 sites.

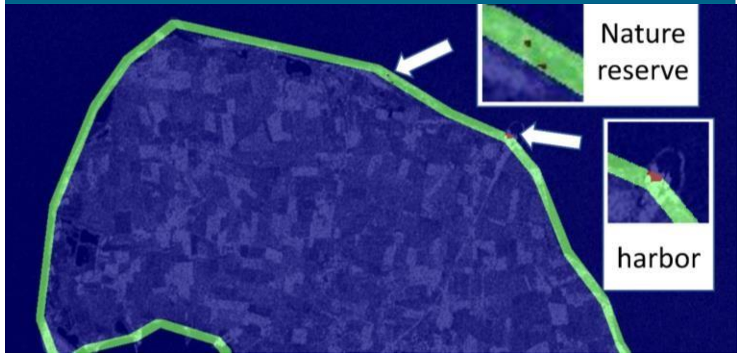
Offices in Brussels, Paris,

Tokyo and Washington.

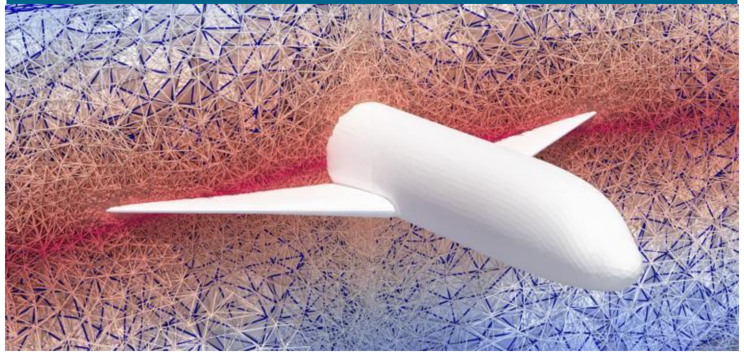
Topic Areas at the Institute of Software Technology (SC)

Dependable, Safe and Secure Software Systems

Artificial Intelligence



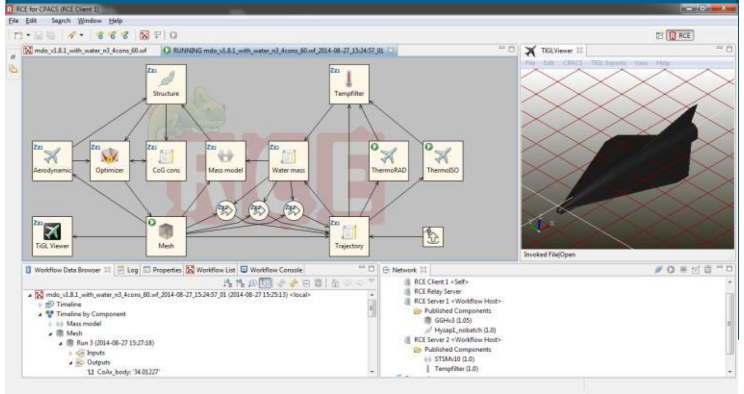
High Performance Computing and Quantum Computing



Human-System-Interaction and Visualisation

Software and Systems Engineering

Digital Platforms



The Institute of Software Technology

Institute of Software Technology

- High-Performance Computing
- Intelligent and Distributed Systems
- Visual Computing and Engineering
- Flight Software

Quantum Computing Methods and Implementations

- Quantum error correction & mitigation
- (Hardware-specific) Compilation
- Circuit optimization
- Realistic noise models
- Hybrid (classical & quantum) computing

Quantum Computing Applications

- Quantum simulation
- Variational quantum algorithms
- Combinatorial optimization with quantum computers
- Mapping of optimization problems onto quantum annealers

Performance Engineering for Mathematical Software

Predictive Simulation Software

Scalable Machine Learning

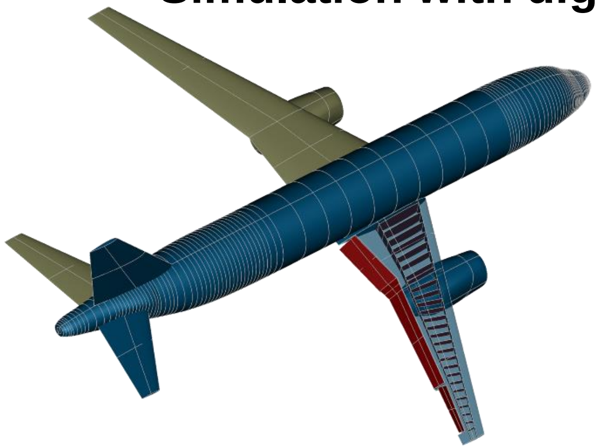
Scientific Machine Learning

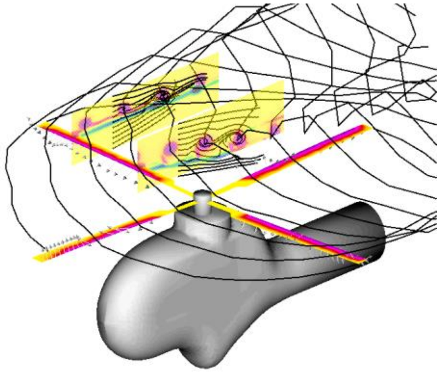
Scalable Adaptive Mesh Refinement

Simulation and Optimization of Technical Systems

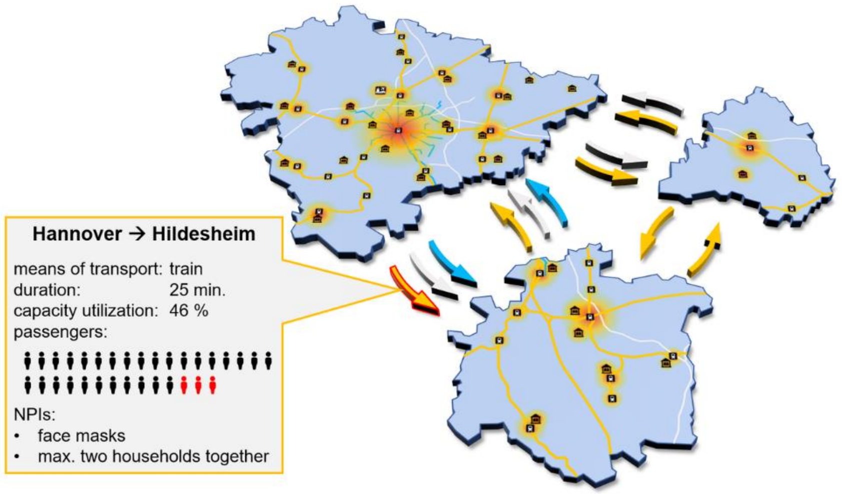
SC-HPC beside Quantum Computing (QC): Data Analysis and Simulation

Simulation with digital twins



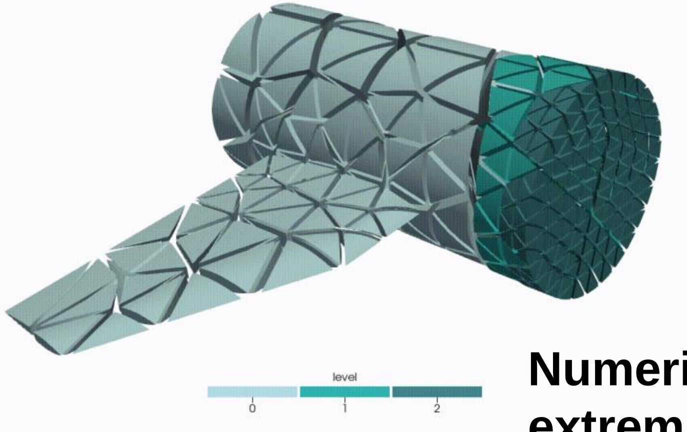


Performance engineering



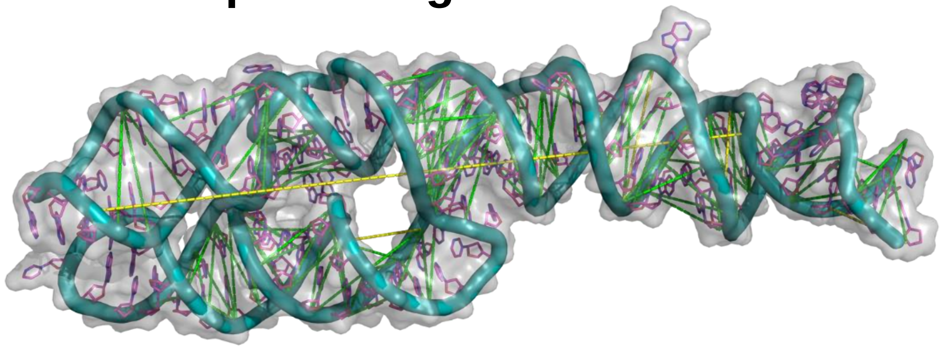
High performance data analytics

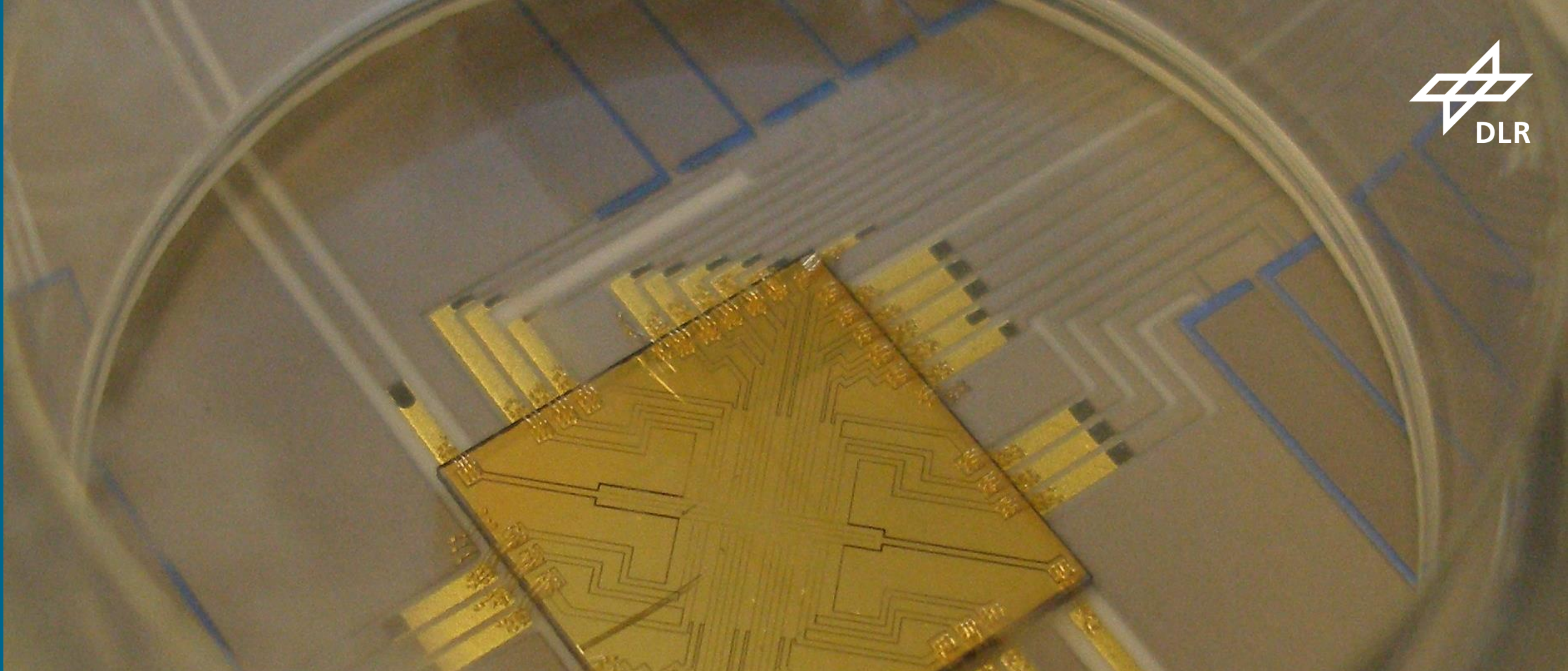
Geometry modelling and form optimization



Numerical simulations with extremly scalable adaptive mesh refinement

Predictive software frameworks based on statistical modelling and deep learning





THE DLR QUANTUM COMPUTING INITIATIVE

DLR Quantum Computing Initiative

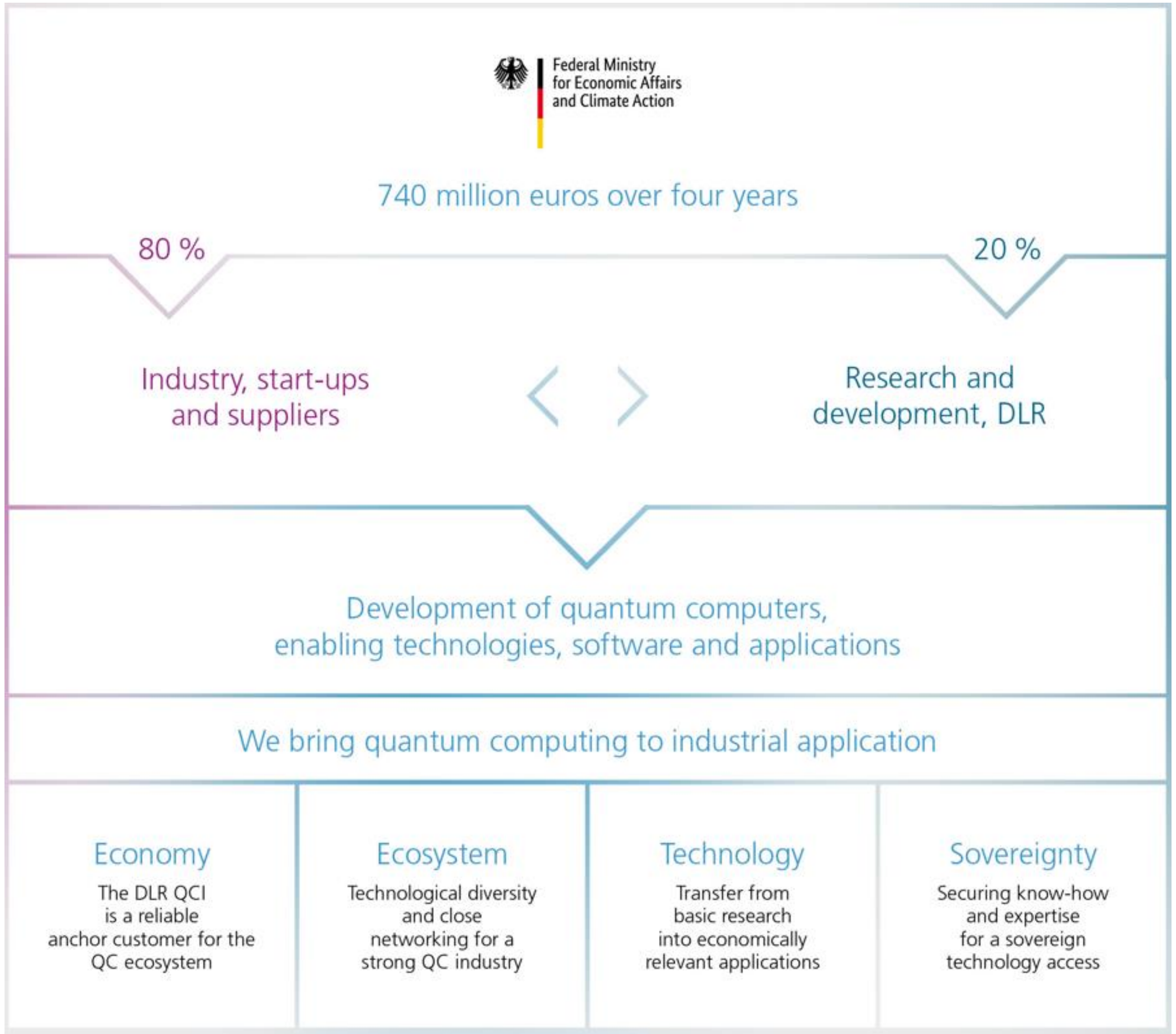
We shape the quantum computing ecosystem

Industry and research jointly develop
Quantum computers, applications & enabling technologies

Financed by 740 million euros from the BMWK
80 percent industry × 20 percent DLR research

Two innovations centers in Hamburg und Ulm
Bundled technology, expertise & infrastructure

We bring quantum computing into application
Currently 5 QC platforms, 17 hardware and 22 software and application projects, 20+ industry commissions



DLR

Hardware

Quantencomputer

- **Legato** – Ionenfallen – Universal Quantum
- **QSea I** – Ionenfallen – eleQtron | ParityQC | NXP
- **QSea II** – Ionenfallen – eleQtron | ParityQC | NXP
- **REDAC** – Analogrechner – Anabrid
- **SuNQC** – NV-Zentren – SaxonQ
- **Toccata** – Ionenfallen – Universal Quantum
- **UPQC** – Photonen – QuiX Quantum
- **XAPHIRO** – Ionenfallen – QUDORA Technologies
- **XQi** – NV-Zentren – XeedQ
- **DiNAQC** – Neutralatome – planqc

Enabling-Technologien

- **DIAQ** – Spin-enabling – Diatope
- **PiQ** – Photonen-enabling – DLR OS
- **SQuAp** – Spin-enabling – Advanced Quantum
- **StarQ** – Spin-enabling – DLR QT
- **TeufIQ** – Spin-enabling – DLR QT

Hardwarenahe Software

- **ALQU** – HW/SW-Kodesign – DLR SC
- **AQuRA** – Analoger Quantenrechner – DLR QT
- **CLIQUE** – QC-Fernzugriff – DLR SC | SP
- **IQDA** – Hardware-nahe Software – DLR SC

Middleware

- **Quant²AI** – Quanten-Maschinelles-Lernen – DLR KI
- **QuTeNet** – Quanten-Maschinelles-Lernen – DLR KI
- **R-QIP** – Quantenfehlerkorrektur – DLR KN | SC | QT | RB

Anwendungen

Anwendungsprojekte

- **Attraqt'em** – Optimierung – DLR VE
- **BASIQ** – Materialwissenschaft – DLR TT
- **Klim-QML** – Quanten-Maschinelles-Lernen – DLR PA
- **QCMobility** – Optimierung – DLR QT | VF | LV | TS | SE
- **QCoKaIn** – Quanten-Maschinelles-Lernen – DLR DW
- **Qlearning** – Quanten-Maschinelles-Lernen – DLR QT
- **QMPC** – Optimierung – DLR RB
- **QUA-SAR** – Optimierung – DLR HR
- **QuantiCoM** – Materialwissenschaft – DLR WF | MP | TT
- **Quantity** – Quanten-Kryptoanalyse – DLR KN
- **ToQuaFlics** – Quanten-Maschinelles-Lernen – DLR AS | SP
- **NeMoQC** – Quanten-Maschinelles-Lernen – DLR KI
- **QC Mineral** – Materialwissenschaft – DLR MP
- **QCOptSens** – Optimierung – DLR OS
- **QI-Mozart** – Optimierung – DLR AS

39 projects for quantum hardware, software & apps

qci.dlr.de

LinkedIn

QCI Details

- 80% for industry partners, 20% for DLR projects
- Research and development on the basis of DLR areas of competence
- Procurement of complete QC systems and components through open-technology competitive tenders
- DLR projects cover 100% of costs, focus on hardware, software, applications and the ecosystem
- Projects with a project volume of several hundred million euros are underway

39 Projects Hardware, Software & Applications

2 Innovation centers in Hamburg | Ulm

11 Quantumcomputer -projects

19 DLR-Institutes

5 Qubit-Platforms

22 Industry partners

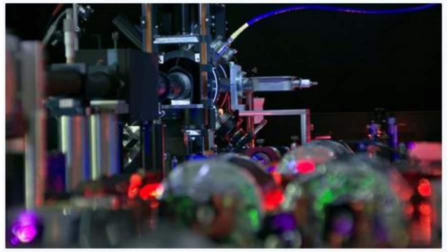
5 Enabling-Technologies

1 Worldwide unique ecosystem

Innovation Center Hamburg

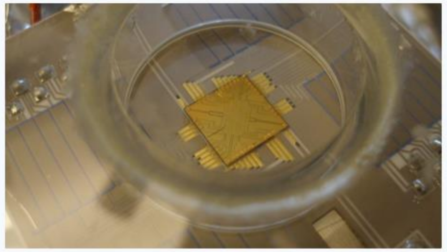
A unique ion trap ecosystem

DLR



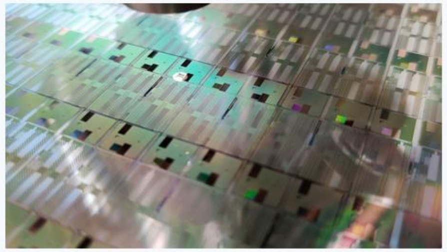
QSea I

■ Ionenfallen ■ Quantencomputer



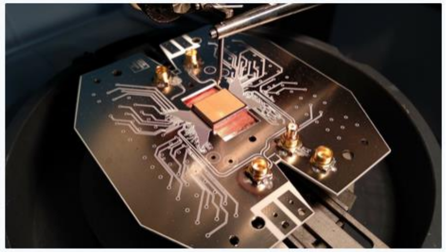
QSea II

■ Ionenfallen ■ Quantencomputer



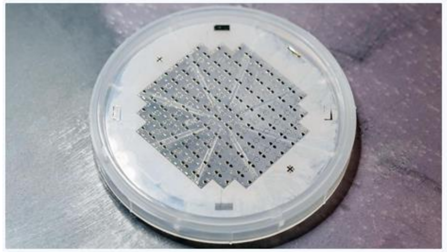
Legato

■ Ionenfallen ■ Quantencomputer



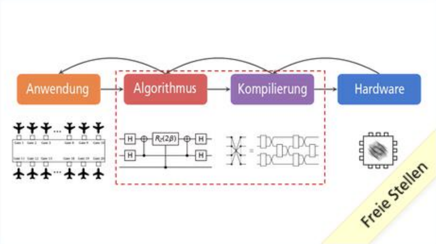
Toccata

■ Ionenfallen ■ Quantencomputer



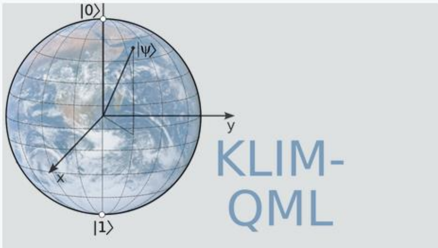
XAPHIRO

■ Ionenfallen ■ Quantencomputer



ALQU

■ Anwendungen ■ HW/SW-Codesign



Klim-QML

■ Anwendungen ■ Quanten-Maschinelles-Lernen

TeuflQ

■ Enabling-Technologien ■ Ionenfallen

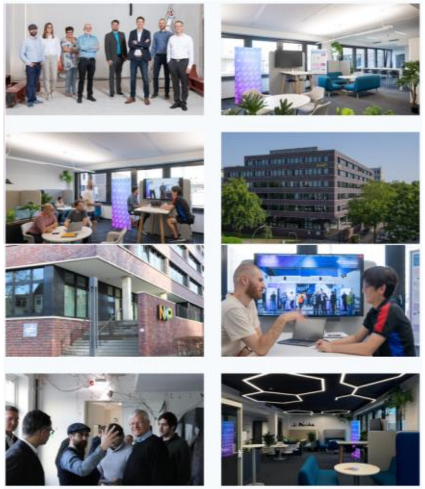
6
Hardware Projekte

5
Auftragnehmer HW, SW, Apps

1.640 m²
Labore, Reinräume, Büros & Coworking

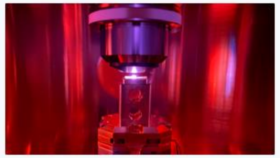
Adresse
Beiersdorfstraße 12
22529 Hamburg

Management
Alain Pierrot



Innovation Center Ulm

A varied ecosystem at the Obere Eselsberg



COMIQC
Customized Organic Molecules for Quantum Computing

- Festkörper-Spin
- Quantencomputer

DiNAQC
Digitaler Neutralatom-Quantencomputer

- Neutralatome
- Quantencomputer

PiQ

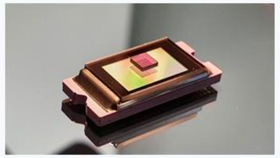
PiQ
Photonenquelle für integrierte Quantenprozessoren

- Enabling-Technologien
- Photonen

StarQ

StarQ
Surface Treatment at Atomic Resolution for Quantum Computing

- Enabling-Technologien
- NV-Zentren



XQi
Quantencomputer auf Basis von NV-Zentren in Diamanten

- NV-Zentren
- Quantencomputer

DiaQ
Diamantmaterial für Raumtemperatur-Quantencomputer

- NV-Zentren
- Spin-enabling Technologien

SQuAp
Spin-Qubit-Analyseplattform für Farbzentren-basierte Quantenhardware

- Enabling-Technologien
- NV-Zentren

SuNQC
Quantencomputer auf Basis von NV-Zentren in Diamanten mit Schwefeldotierungen

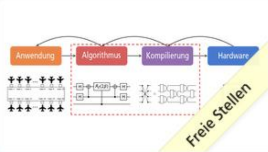
- NV-Zentren
- Quantencomputer

UPQC
Universeller photonischer Quantencomputer mit bis zu 64 Qubits

- Photonen
- Quantencomputer

REDAC
Reconfigurable Discrete Analog Computer

- Analogrechner
- Computer



ALQU
Algorithmen für Quantencomputer-Entwicklung im Hardware-Software-Codesign

- Anwendungen
- HW/SW-Codesign

AQuRA

AQuRA
Ein analoger Quantenrechenautomat

- Analoger Quantenrechner
- Hardware-nahe Software

9 Hardware Projekte

8 Auftragnehmer HW, SW, Apps

1.590 m^2 Labore, Reinraum, Büros & Coworking

Adresse
Wilhelm-Runge-Straße 10
89081 Ulm

Management
Kathrin Höppner







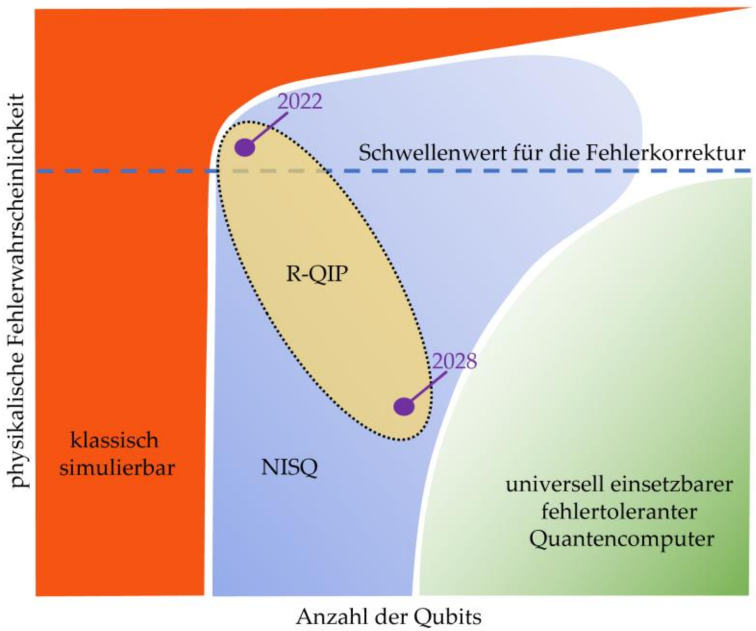

Industry Partners

DLR

Advanced Quantum | anabrid | diatope | e·on | d-fine | eleQtron | Fraunhofer ITWM

HQS Quantum Simulations | IQM | Kipu Quantum | Multiverse Computing | NVISION | NXP | parityqc

planqc | Qudora Technologies | QuiX Quantum | Universal Quantum | SaxonQ | Single Quantum Excellence in photon detection | XEED



R-QIP

Reliable Quantum Information Processing

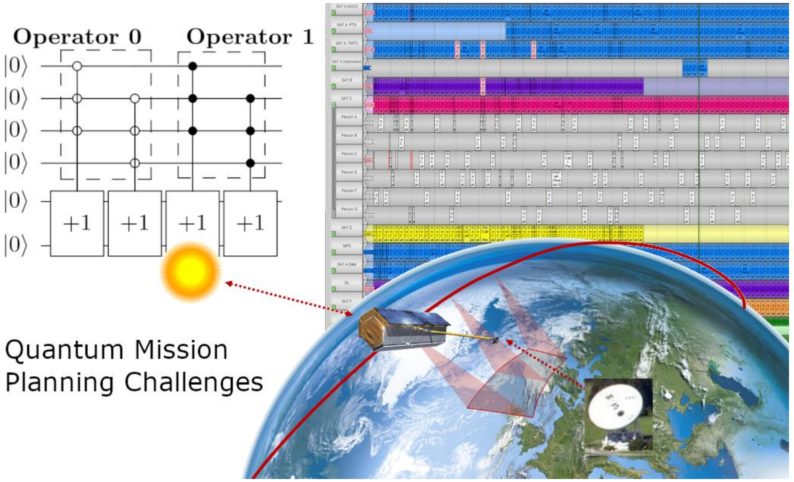
Enhancing the reliability of quantum information processing with novel error models, simulators for quantum error correction and new quantum decoders

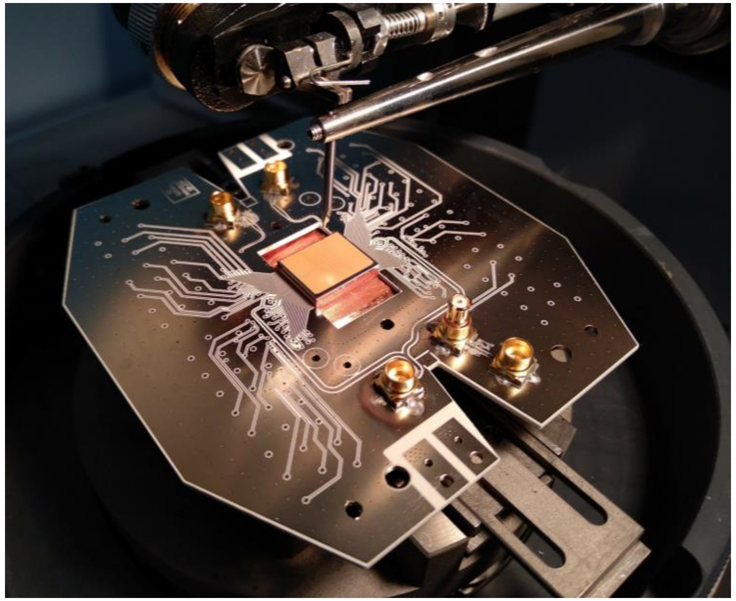
QMPC

Quantum Mission Planning Challenges

Solving mission planning problems with quantum algorithms and creating an interface between classical and quantum planning tools

Contractor: E.ON

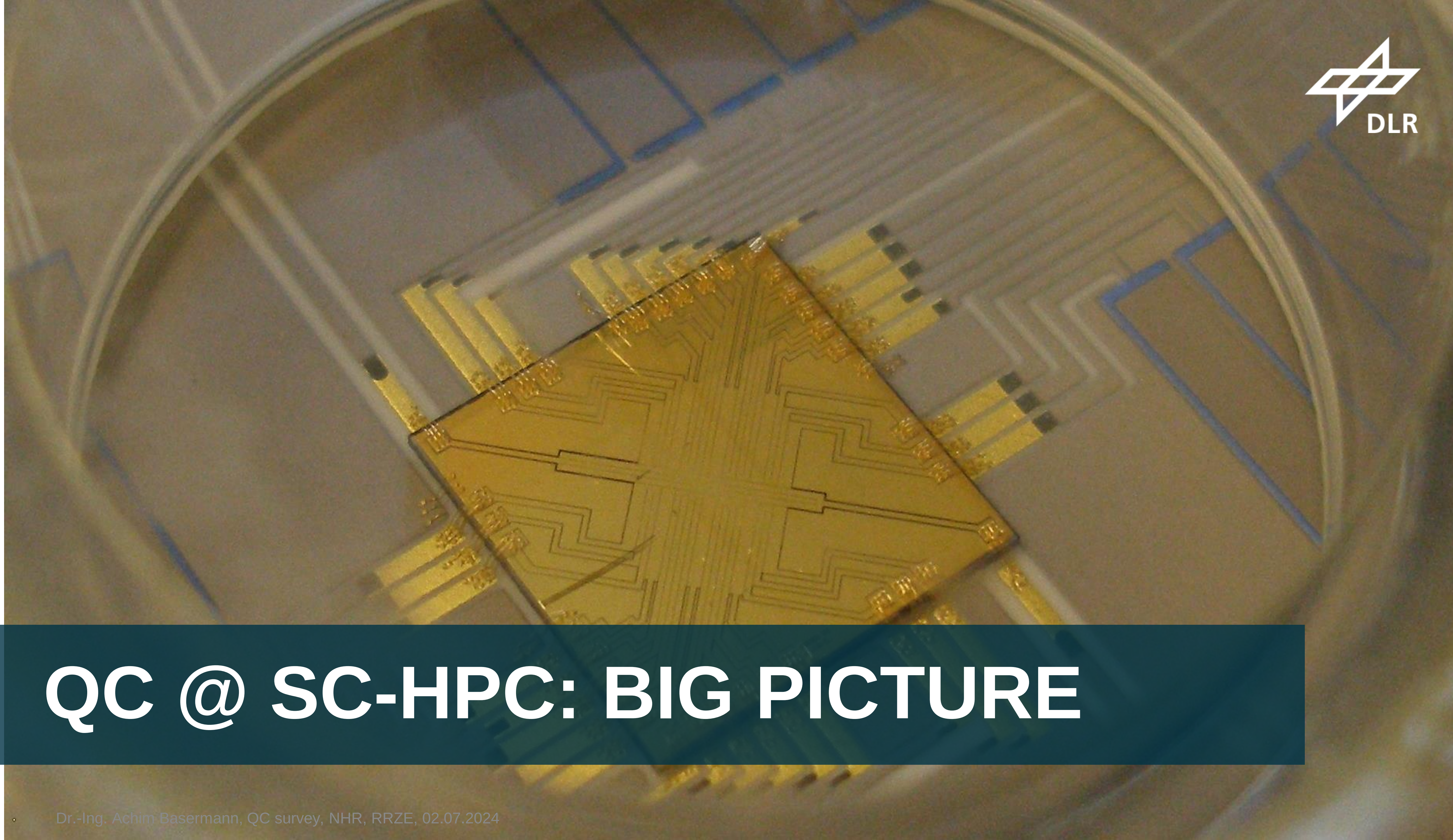




Toccata

Building a user-friendly, reliable and scalable quantum processor with 50+ qubits on the basis of ion trap technology

Contractor: Universal Quantum



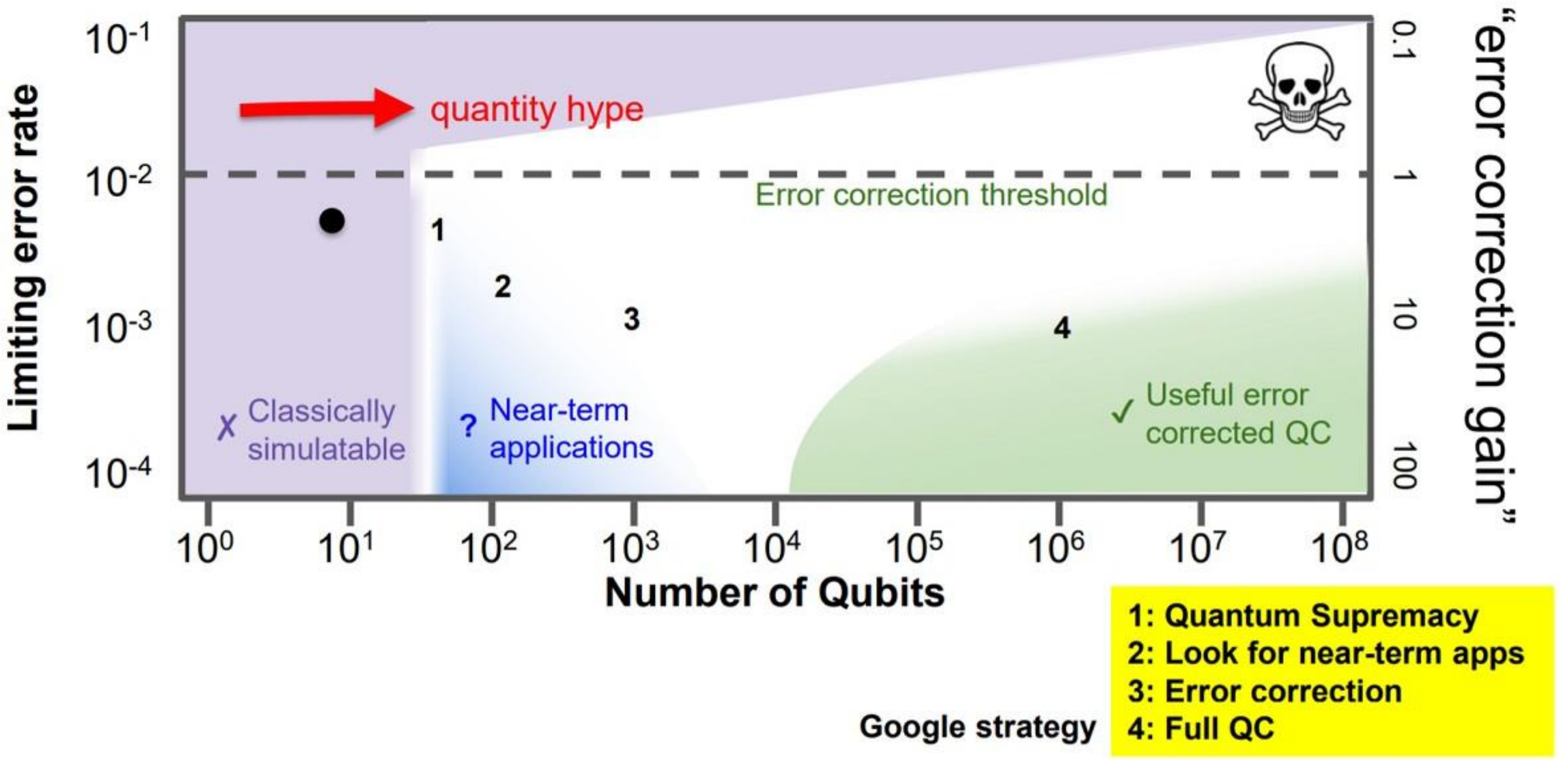
QC @ SC-HPC: BIG PICTURE

Background: Development Status Quantum Computers

Cf. BSI study to the development status of quantum computers: https://www.bsi.bund.de/qcstudie

Quantum error correction (QEC)

- Univeral quantum comuters are intrinsically error prone. For the implementation of *killer apps* (e.g. Shor) we therefore need QEC.
- QEC bases on redundancy. Thus QEC generates a significant overhead in required qubits and gates.

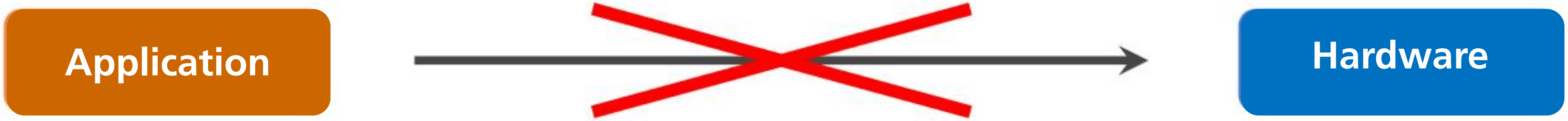


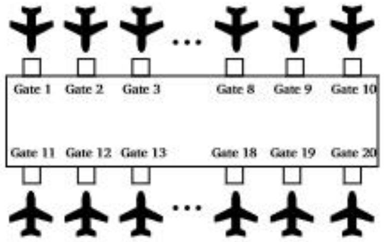
If we want to achieve quantum supremacy for a real world problem in the near future then only with NISQ computers!

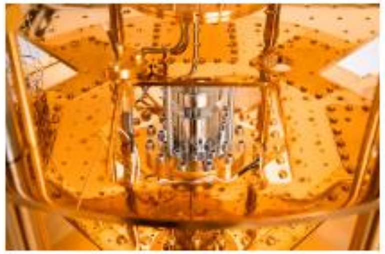
Picture: John Martinis, Google. (taken from https://medium.com/@quantum_wa/quantum-computing-near-and-far-term-opportunities-f8ffa83cc0c9)

Noisy Intermediate-Scale Quantum Devices (NISQ)

- State-of-the-art quantum computers are usually small, noisy and have a limited connectivity.
- In the coming years we expect quantum computers without complete QEC.
- Is it still possible to achieve quantum supremacy or at least a distinct quantum advantage?



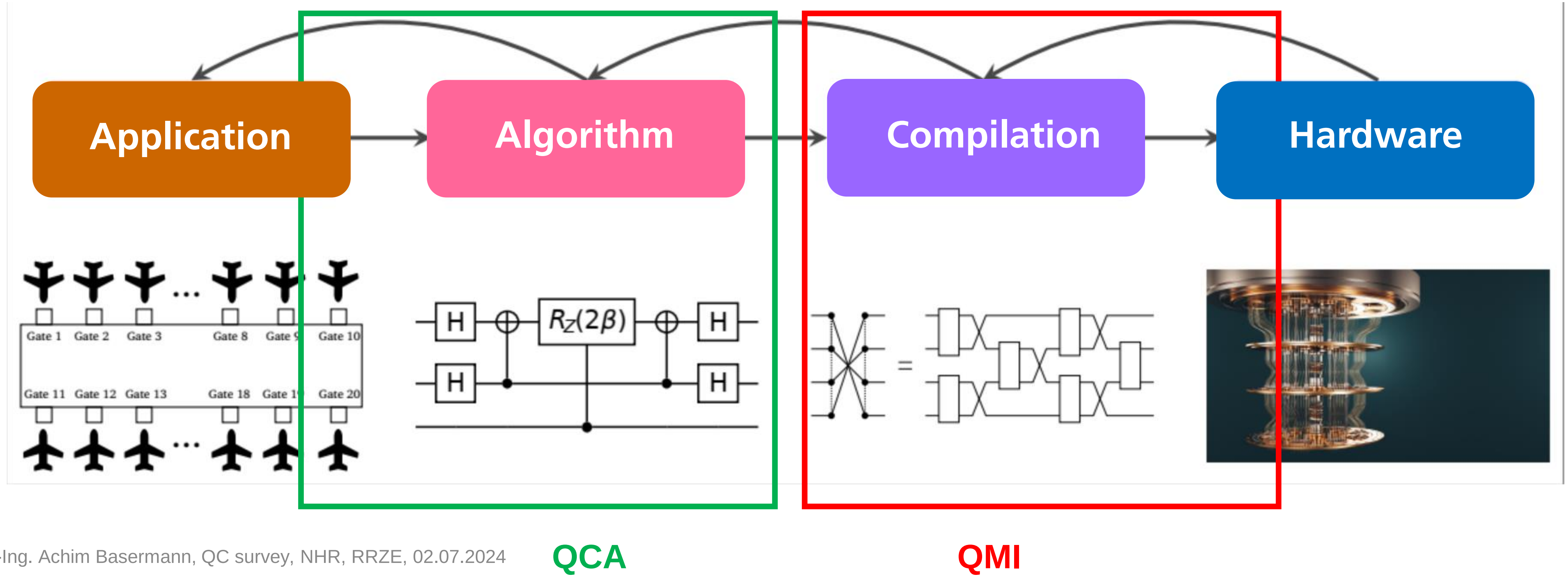




Hardware-Software Codesign

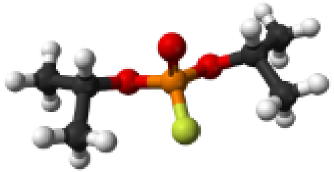
In order to achieve quantum supremacy we should …

- … observe the hardware evolution with respect to potential applications and
- … consider error correction/mitigation for all software developments due to the erroneous and limited current hardware.

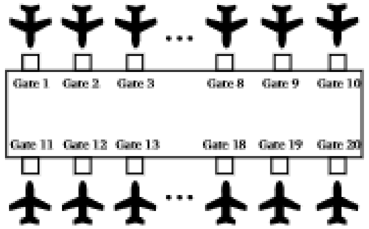


Which are promising applications?*

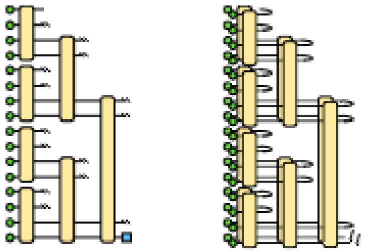
quantum simulation



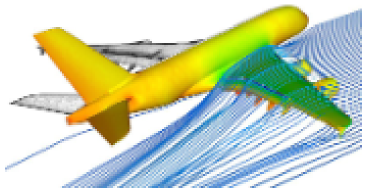
combinatorial optimization



quantum accelerated ML



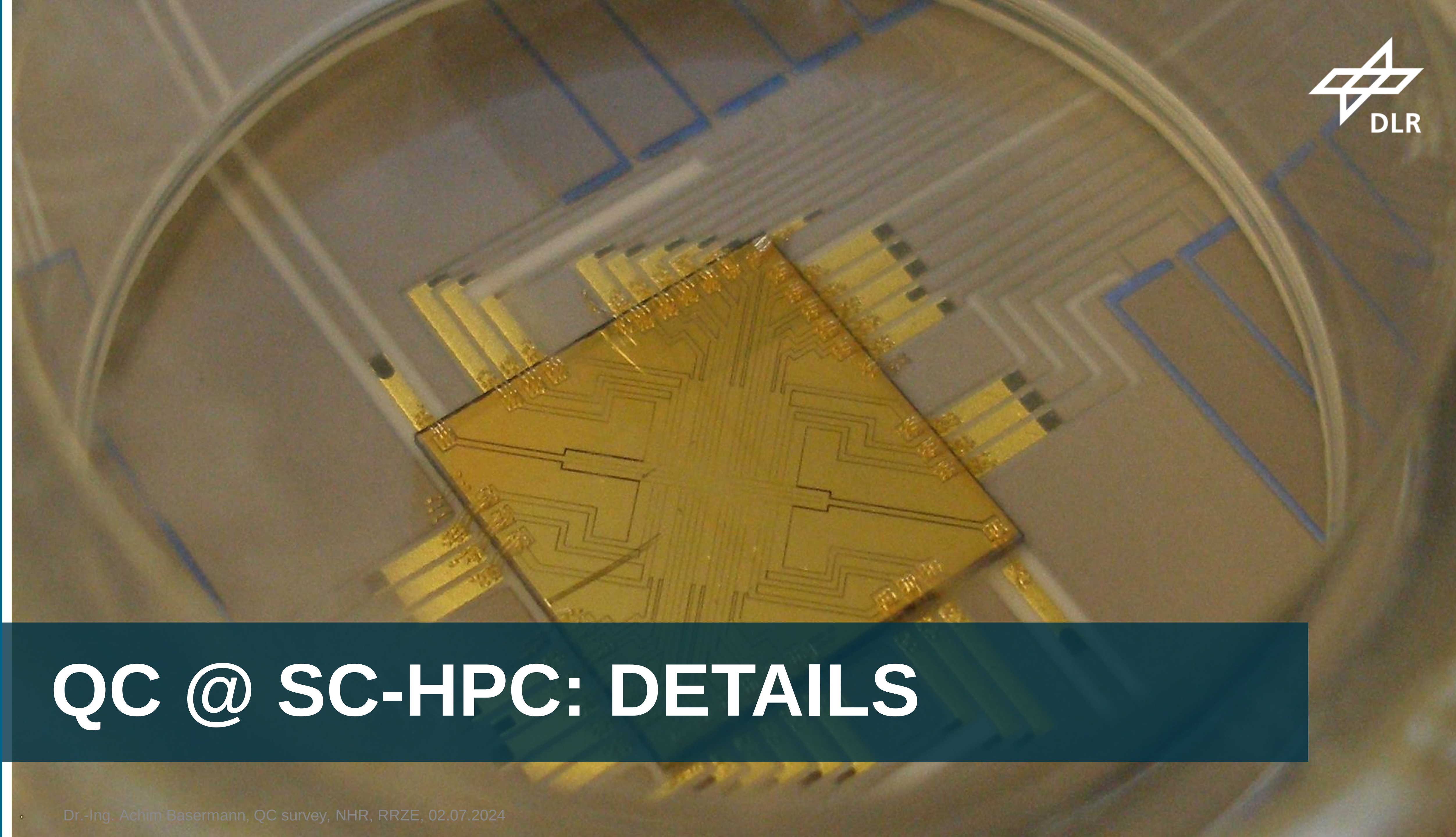
classical simulation



Today

Time / required quantum error correction

*Own judgement with no guarantee



QC @ SC-HPC: DETAILS

Two Entangled Sites

- Konrad-Adenauer Stiftung in Sankt Augustin
- Recently moved here

- Innovation Center in Hamburg-Lokstedt
- One of two sites where our QC are built

Quantum Computing Methods and Implementations (QMI)


Michael
Epping


Pedro
Barrios


David
da Costa


Joseph
Harris


Alexander
Kegeles


Thomas
Keitzl


Thorge
Müller


Vittorio
Pagni


Johannes
Renkl


Linus
Scholz


Peter
Schuhmacher


Thomas
Stehle


Yoshinta
Wied


Christian
Wimmer

Quantum Computing Activities

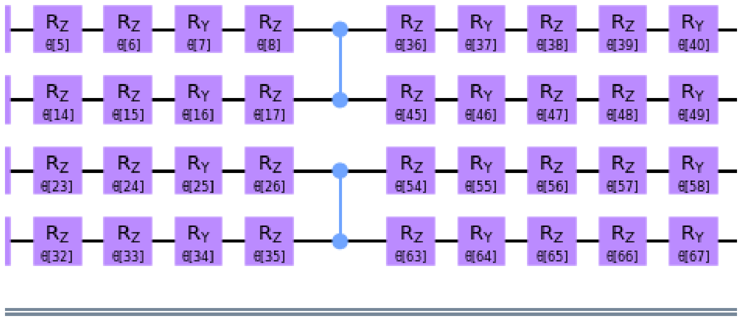
Some of our partners

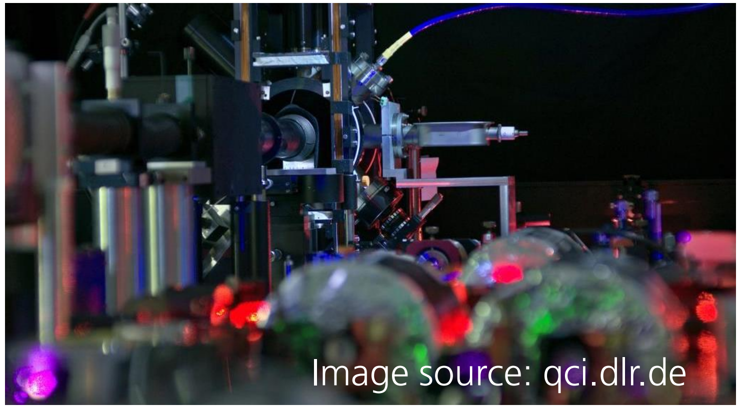
- DLR projects
  - ALQU/CLIQUE: Compilation, error correction, integration
  - R-QIP: Error correction, error mitigation
  - ELEVATE: Training of other DLR institutes and evaluation of their use-cases
  - Several PhD projects
- EU projects
  - EQUIP: Error correction
  - EQUALITY: Industrial use cases, hardware exploitation
    our part: compilation, routing
- BMWK projects
  - AQUAS: Quantum simulation for hydrogen generation

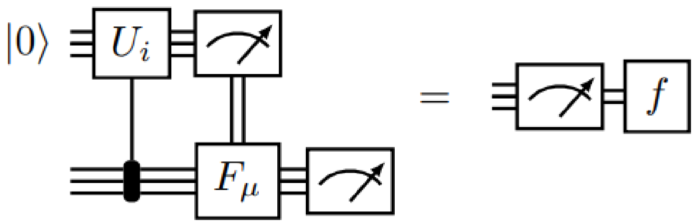
Research Activities: Compiling for our Quantum Computers

Several projects – one compiler

Circuit optimization	Hardware-specific	QPUs as accelerators







Circuit optimization

- Reduce number of gates
- For small/special circuits find optimal solution
- Take noise into account

Hardware-specific

- Output only gates native to the machine
- Exploit features like multi-qubit operations

QPUs as accelerators

- Use quantum computer only for coherent computations
- Develop techniques for hybrid programming

Research Activities: Software Stack and QC Integration

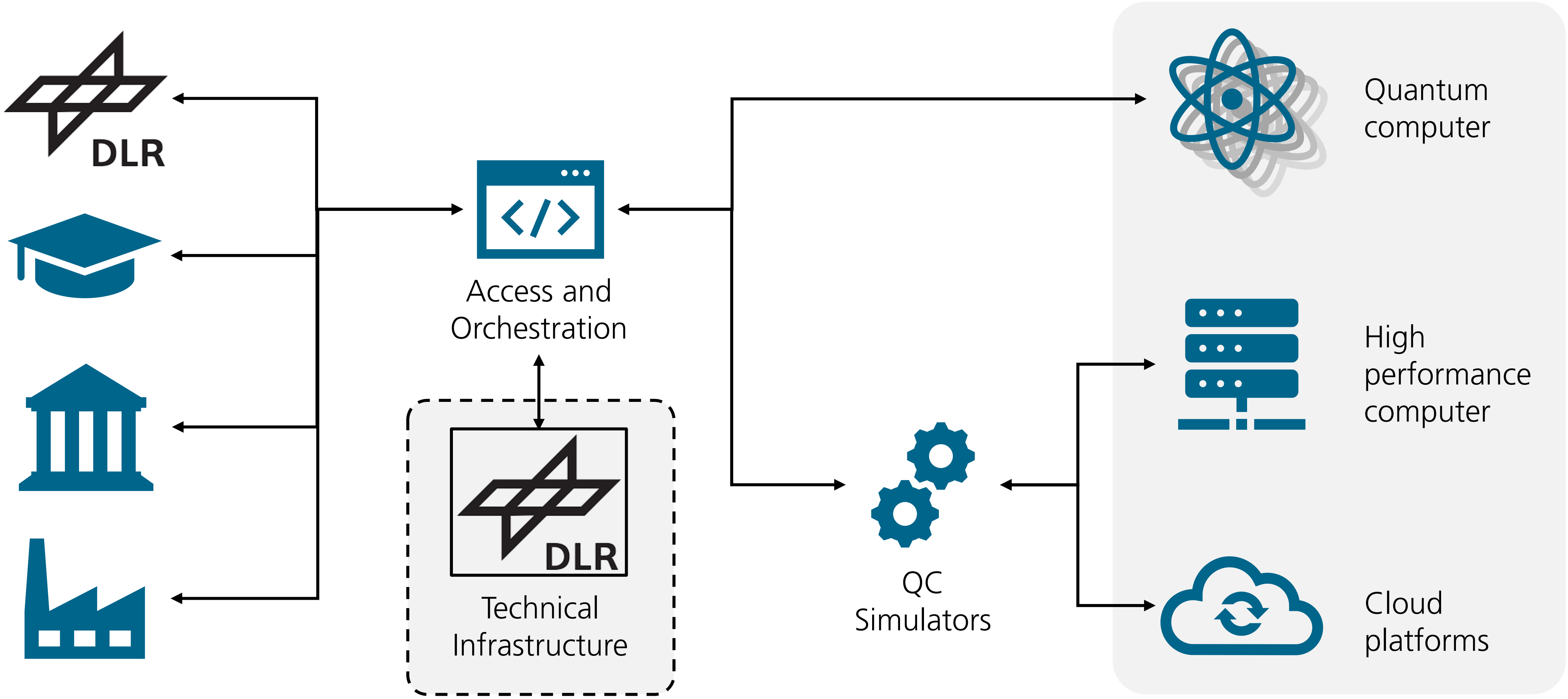
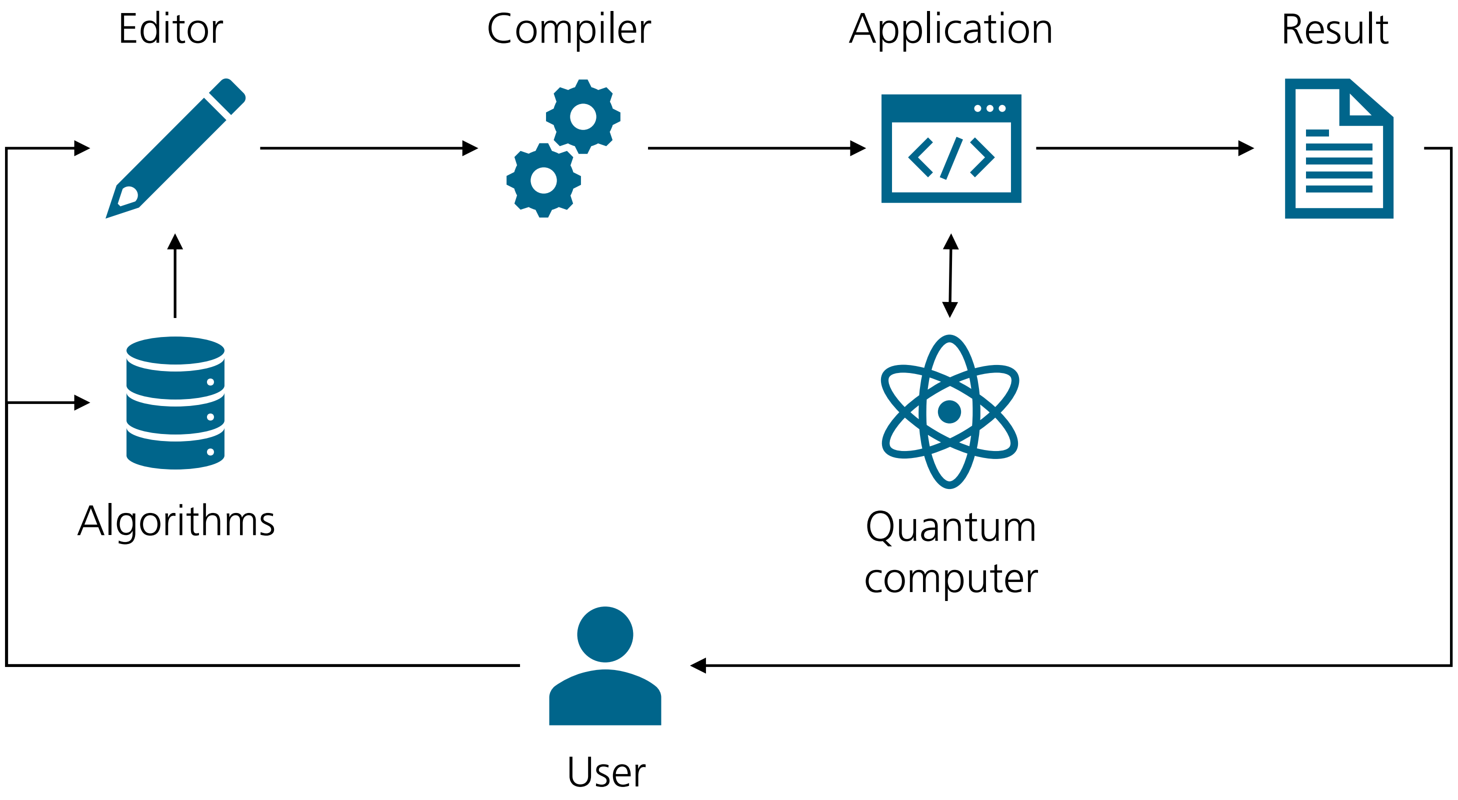


Image source: https://qci.dlr.de/posterpraesentationen/

Research Activities: Software Stack and QC Integration

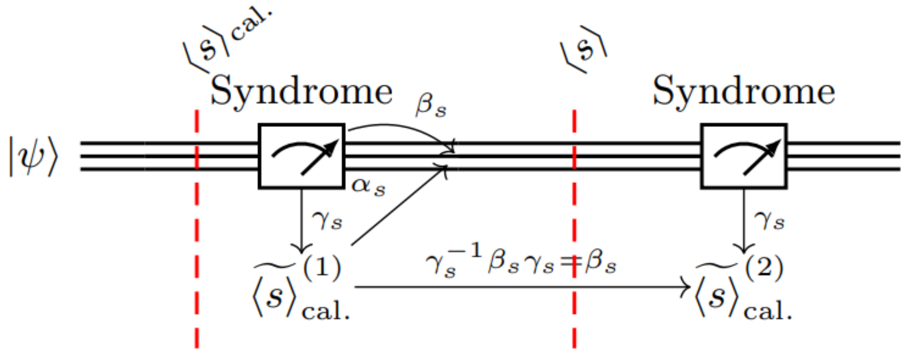


- We work together with industrial partners on
  - Unified interfaces for different QC hardware
  - Integration of state-of-the-art compilation techniques into tool chain
  - Analysis of the outcome statistics (QC result)

Image source: https://qci.dlr.de/posterpraesentationen/

Research Activities: Mitigate noise

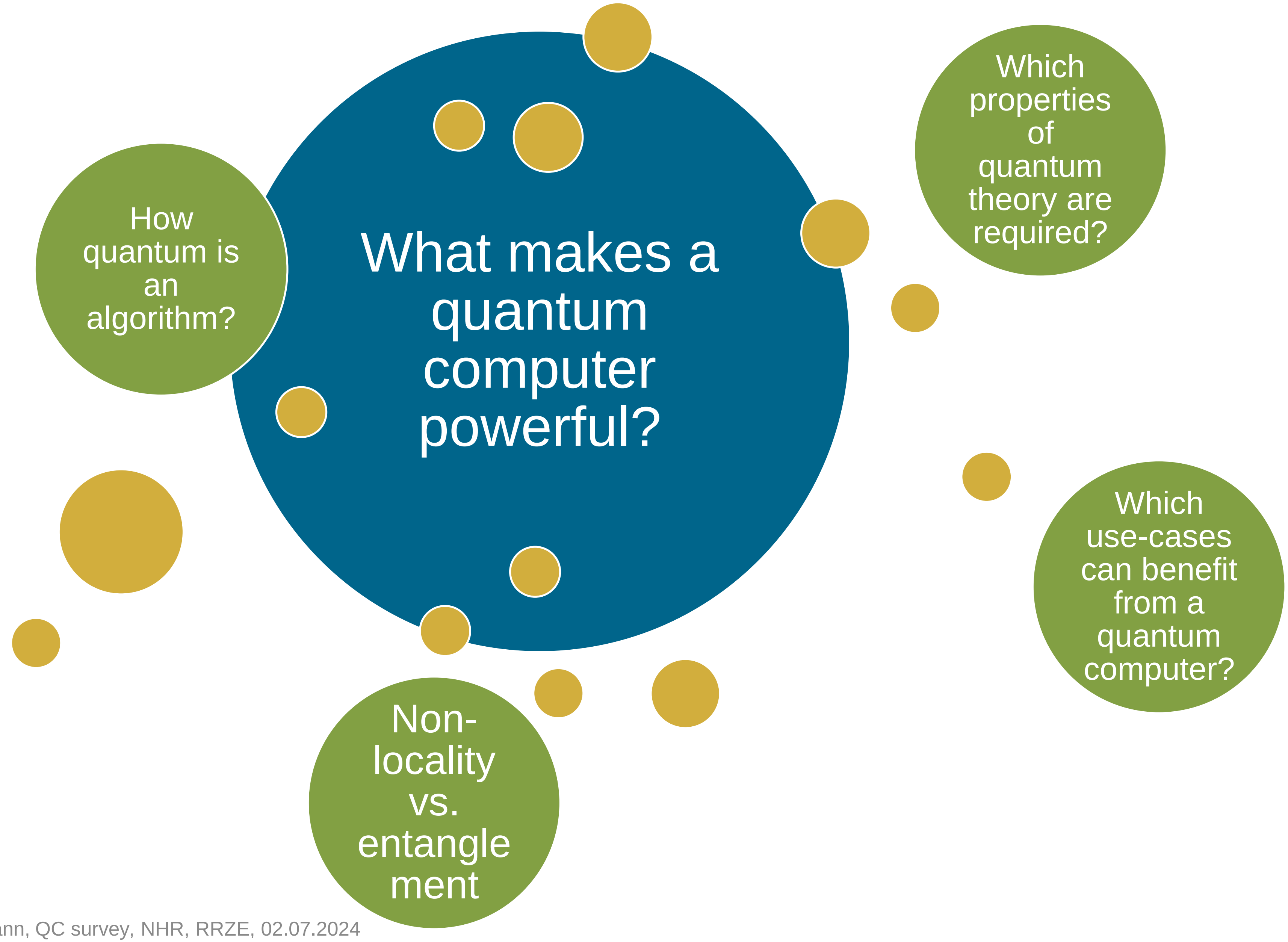
- Calibration of syndrome measurements



- Improves error correction, noise estimation
- Also interested in
  - Benefits of small error correction codes
  - Application-taylored quantum error correction

Image source: arXiv:2305.03004 [quant-ph]

Research Activities: Understanding Quantum Advantage



Research Activities: Testing of Quantum Software

- Assertions are difficult in quantum computers, because they affect the state
- Transfer concepts from quantum error correction, e.g. stabilizer measurements
- Apply to crucial basic building blocks, like state preparation
- Develop best practices
- Program verification
- Using QC simulators for comparison
- **QC performance engineering:** performance models, performance test, benchmarking → how to do it best, in particular for hybrid computing?
- Hybrid computing: additional scheduling challenges

Selected Publications

- M. Felderer, D. Taibi, F. Palomba, M. Epping, M. Lochau, and B. Weder, *Software engineering challenges for quantum computing.* ACM SIGSOFT Software Engineering Notes, 48:29 – 32, 2023.
- A. Misra-Spieldenner, T. Bode, P. K. Schuhmacher, T. Stollenwerk, D. Bagrets, and F. K. Wilhelm. *Mean-Field Approximate Optimization Algorithm.* PRX Quantum 4, 030335 (2023)
- T. Müller, T. Stollenwerk, D. Headley, M. Epping, and F. K. Wilhelm. *Coherent and non-unitary errors in ZZ-generated gates.* arXiv:2304.14212 (2023)
- A. A. Buchheit, T. Keßler, P. K. Schuhmacher, and B. Fauseweh. *Exact Continuum Representation of Long-range Interacting Systems and Emerging Exotic Phases in Unconventional Superconductors.* Phys. Rev. Research 5, 043065 (2023)
- C. Wimmer, J. Szangolies, and M. Epping. *Calibration of Syndrome Measurements in a Single Experiment.* arXiv:2305.03004 (2023)
- M. Epping. *Hybrid simplification rules for boundaries of quantum circuits.* arXiv:2206.03036 (2023)
- J. Harris, and E. Kashefi. *Scalable and Exponential Quantum Error Mitigation of BQP Computations using Verification.* arXiv:2306.04351 (2023)
- D. Headley, T. Müller, A. Martin, E. Solano, M. Sanz, and F. K. Wilhelm, *Approximating the quantum approximate optimization algorithm with digital-analog interactions,* Phys. Rev. A **106**, 042446 (2022)

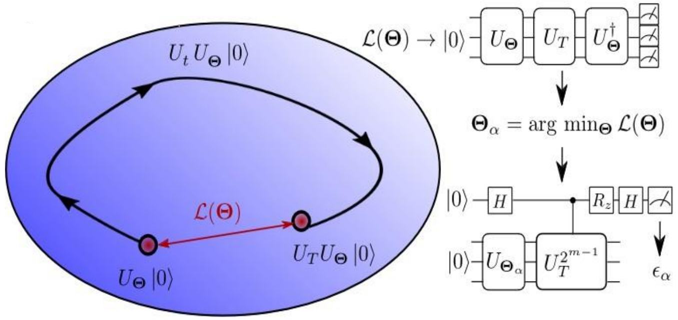
Quantum Computing Applications (QCA)

David Haink, Gonzalo Camacho, Satoshi Ejima, Benedikt Fauseweh, Jonathan Busse, Gary Schmiedinghoff, Elisabeth Lobe (Group Lead), Alina Joch, Kevin Lively, Jochen Szangolies, Fabian Eickhoff, Lukas Windgätter, Bavithra Govintharajah

Research Areas

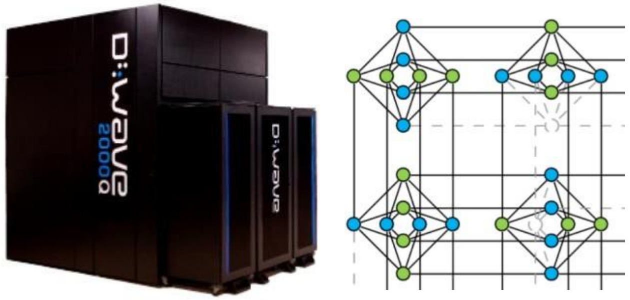
Digital Quantum Simulation

- New algorithms for quantum many body dynamics
- Development of quantum simulation software for NISQ devices



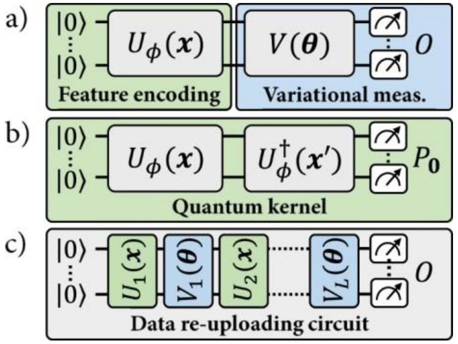
Combinatorial Optimization

- Combinatorial optimization problems around quantum annealers
- Development of open-source software library (quark and Co.)



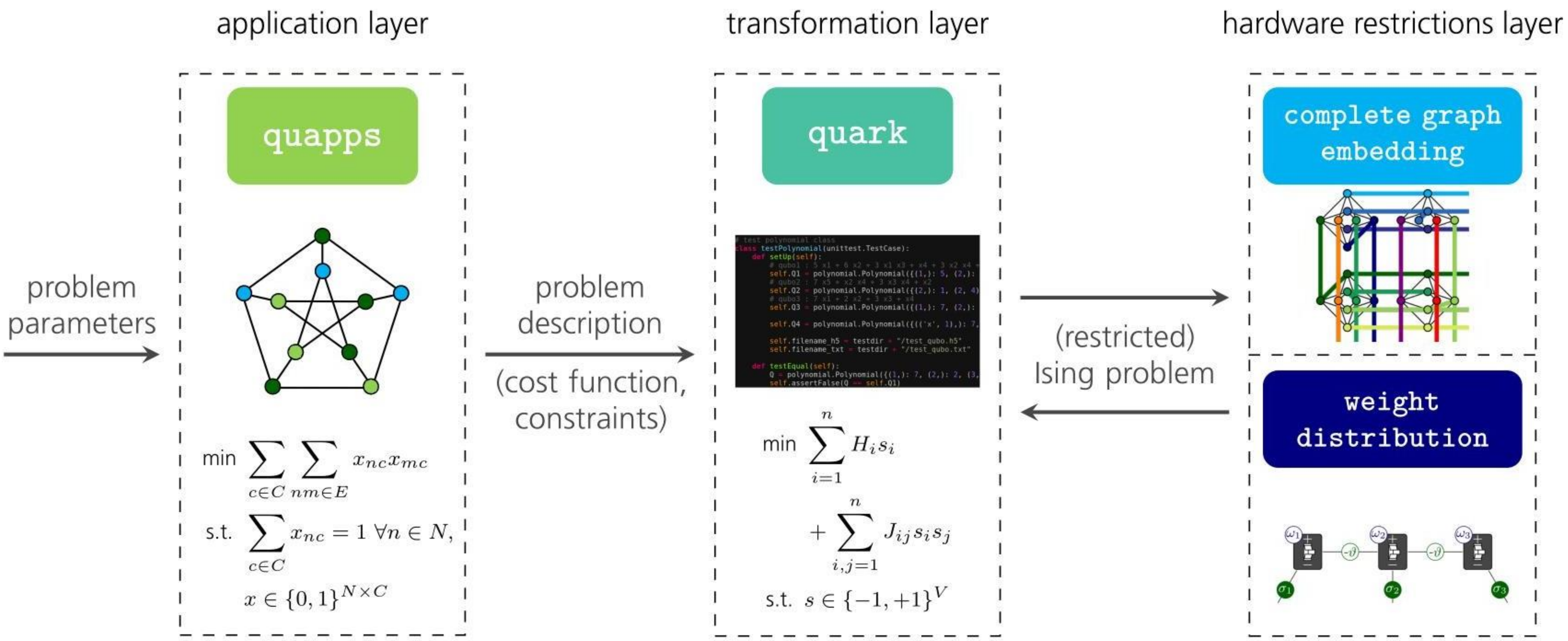
Other Quantum Applications and Quantum-inspired Algorithms

- Quantum machine learning
- Description of new quantum computing platforms (e.g. topological QCs)
- State-of-the-art numerical software for QC benchmarks



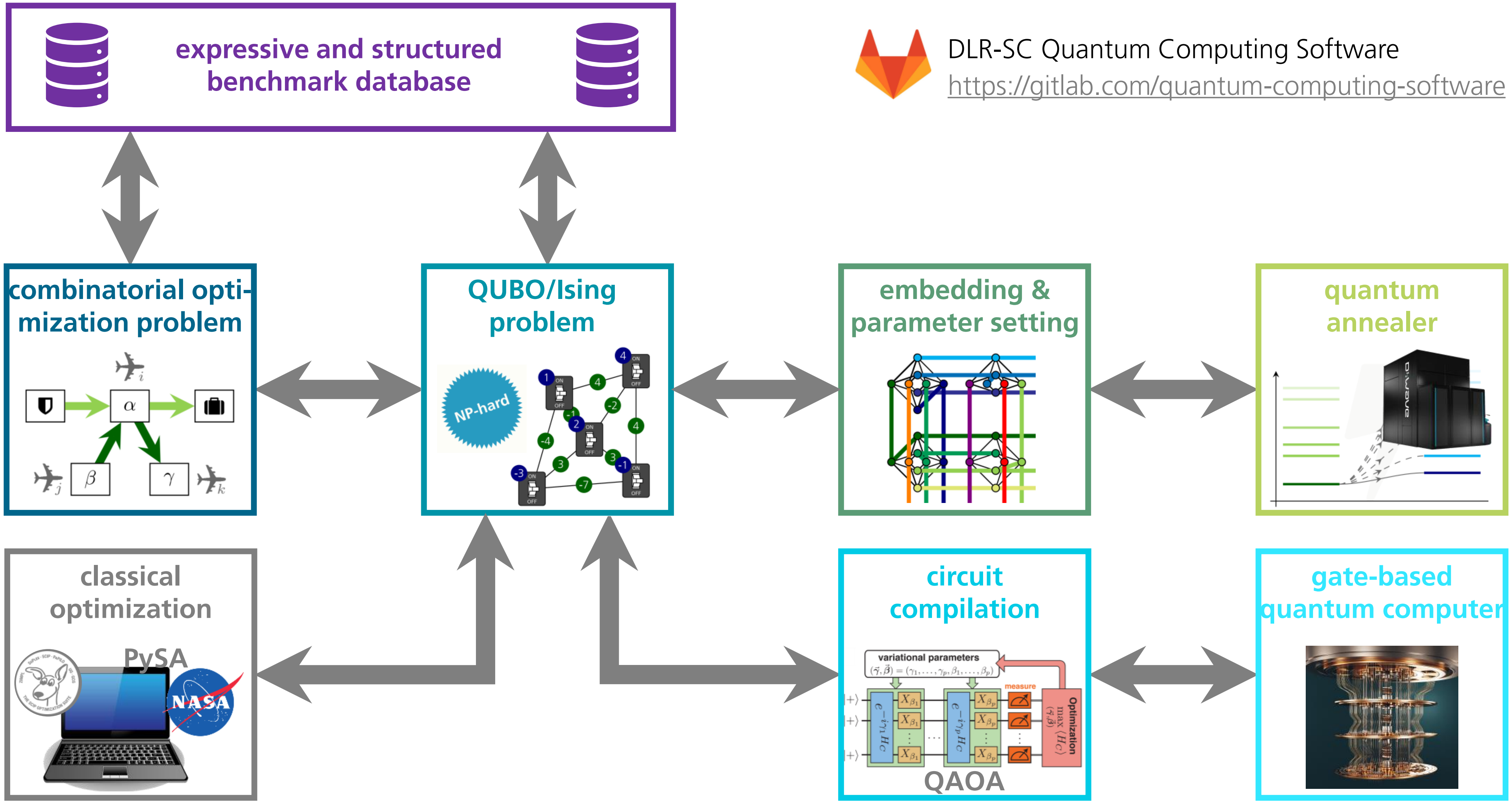
Supported by our Software Library

https://gitlab.com/quantum-computing-software/



Software Framework for Quantum Application Benchmarks

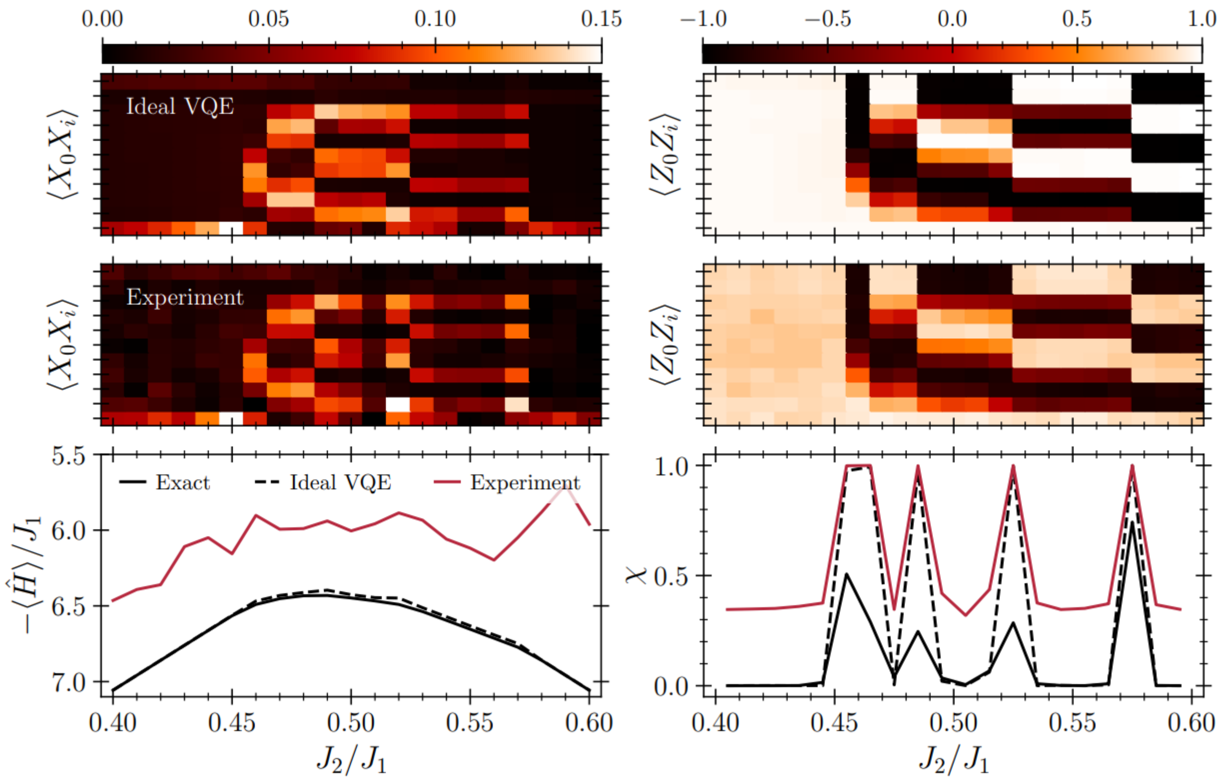
DLR-SC Quantum Computing Software
https://gitlab.com/quantum-computing-software



Robust Experimental Signatures of Phase Transitions in the Variational Quantum Eigensolver

Lively, K., Bode, T., Szangolies, J., Zhu, J. X., & Fauseweh, B., arXiv:2402.18953

- Quantum computers usable for material development require realistic quantum advantage
- Current quantum computers (NISQ) are too noise-prone for many applications
- Error handling techniques are not sufficiently scalable
- Complex systems can still be characterised by selecting noise-robust parameters
- An investigation of corresponding variables can leverage a real quantum advantage with quantum computers available in the near future



Focusing on scalar parameters (energy, bottom left) allows few qualitative conclusions to be drawn about the system. Better use of the data with meaningful variables, on the other hand, can reliably characterise phase transitions.

Scientific Output (2023 – today)

DLR

Published:

- Ejima, Satoshi und Fehske, Holger (2023) *Photoinduced pairing in Mott insulators.* **SciPost Phys. Proc**. doi: 10.21468/SciPostPhysProc.11.009
- Ejima, Satoshi und Lange, Florian und Fehske, Holger (2023) *Entanglement analysis of photoinduced η-pairing states*. doi: 10.1140/epjs/s11734-023-00975-6
- Sugimoto, Koudai and Ejima Satoshi (2023) *Pump-probe spectroscopy of the one-dimensional extended Hubbard model at half filling.* **Phys. Rev. B**. doi: 10.1103/PhysRevB.108.195128
- Fauseweh, Benedikt und Zhu, Jian-Xin (2023) *Quantum computing Floquet energy spectra.* **Quantum**. doi: 10.22331/q-2023-07-20-1063
- Buchheit, Andreas A. und Keßler, Torsten und Schuhmacher, Peter Ken und Fauseweh, Benedikt (2023) *Exact continuum representation of long-range interacting systems and emerging exotic phases in unconventional superconductors*. **Physical Review Research**. doi: 10.1103/PhysRevResearch.5.043065
- Lively, Kevin und Sato, Shunsuke A. und Albareda, Guillermo und Rubio, Angel und Kelly, Aaron (2024) *Revealing ultrafast phonon mediated inter-valley scattering through transient absorption and high harmonic spectroscopies.* **Physical Review Research**. doi: 10.1103/PhysRevResearch.6.013069
- Lobe, Elisabeth und Kaibel, Volker (2023) *Optimal sufficient requirements on the embedded Ising problem in polynomial time*. **Quantum Information Processing**. doi: 10.1007/s11128-023-04058-2
- Lobe, Elisabeth und Lutz, Annette (2023) *Minor Embedding in Broken Chimera and Derived Graphs is NP-complete*. **Theoretical Computer Science**. doi: 10.1016/j.tcs.2023.114369
- Lobe, Elisabeth (2023) `quark`*: QUantum Application Reformulation Kernel*. **INFORMATIK 2023 - Designing Futures: Zukünfte gestalten**, P337, GI Quantum Computing Workshop 2023. doi: 10.18420/inf2023_123.

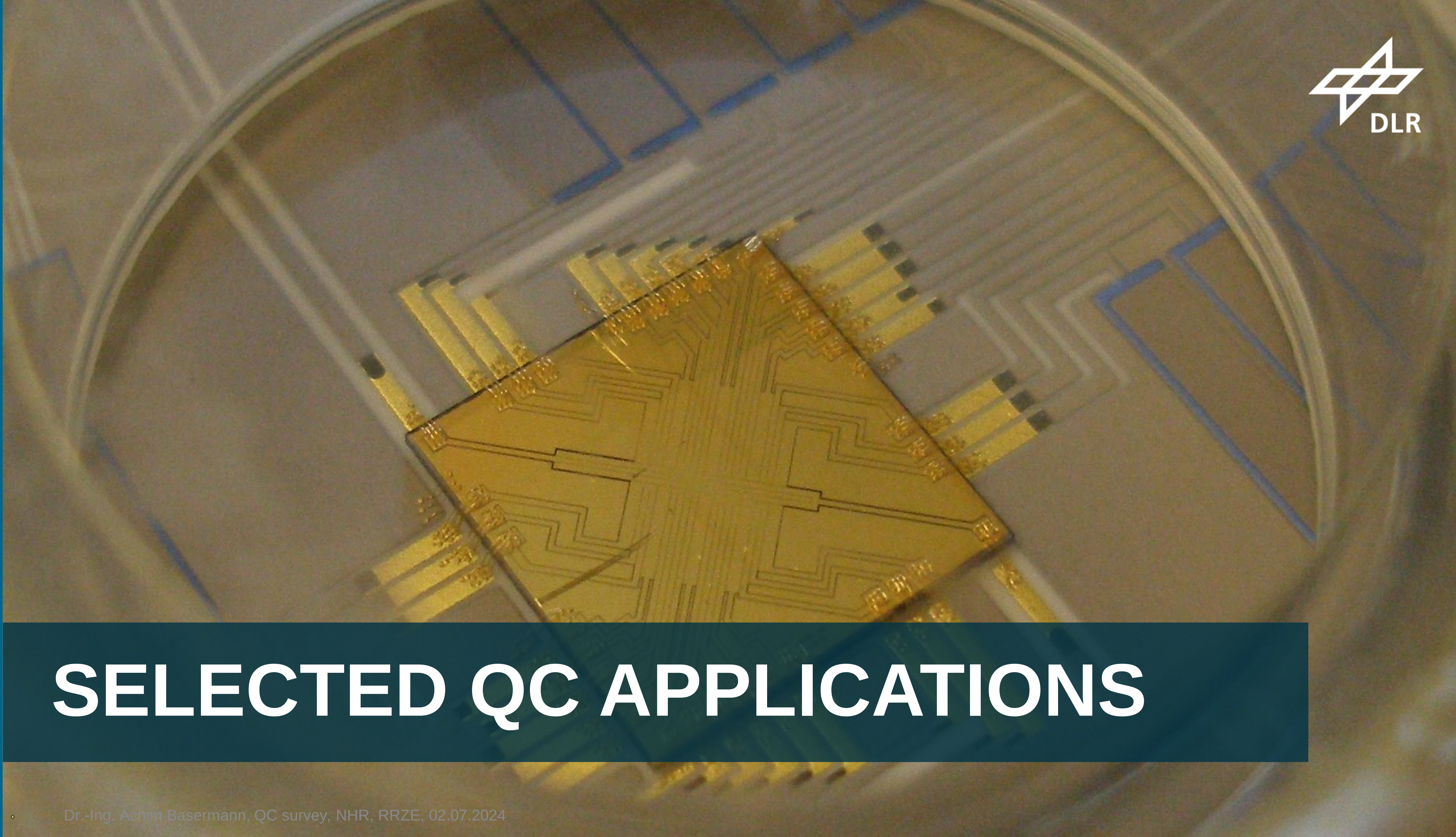
Scientific Output (2023 – today)

Preprints:

- Camacho, Gonzalo und Fauseweh, Benedikt (2023) *Prolonging a discrete time crystal by quantum-classical feedback*. arXiv:2309.02151
- Eickhoff, Fabian und Anders, Frithjof B. (2024) Kondo breakdown in multi-orbital Anderson lattices induced by destructive hybridization interference. arXiv:2401.04540
- Z. Huang, C. Lane, S. E. Grefe, S. Nandy, B. Fauseweh, S. Paschen, Q. Si, J.-X. Zhu (2023) *Dark Matter Detection with Strongly Correlated Topological Materials: Flatband Effect*. arXiv:2305.19967
- Lively, K., Bode, T., Szangolies, J., Zhu, J. X., & Fauseweh, B. (2024). *Robust Experimental Signatures of Phase Transitions in the Variational Quantum Eigensolver*. arXiv preprint arXiv:2402.18953.
- Wimmer, Christian und Szangolies, Jochen und Epping, Michael (2023) *Calibration of Syndrome Measurements in a Single Experiment.* arXiv:2305.03004

Submitted:

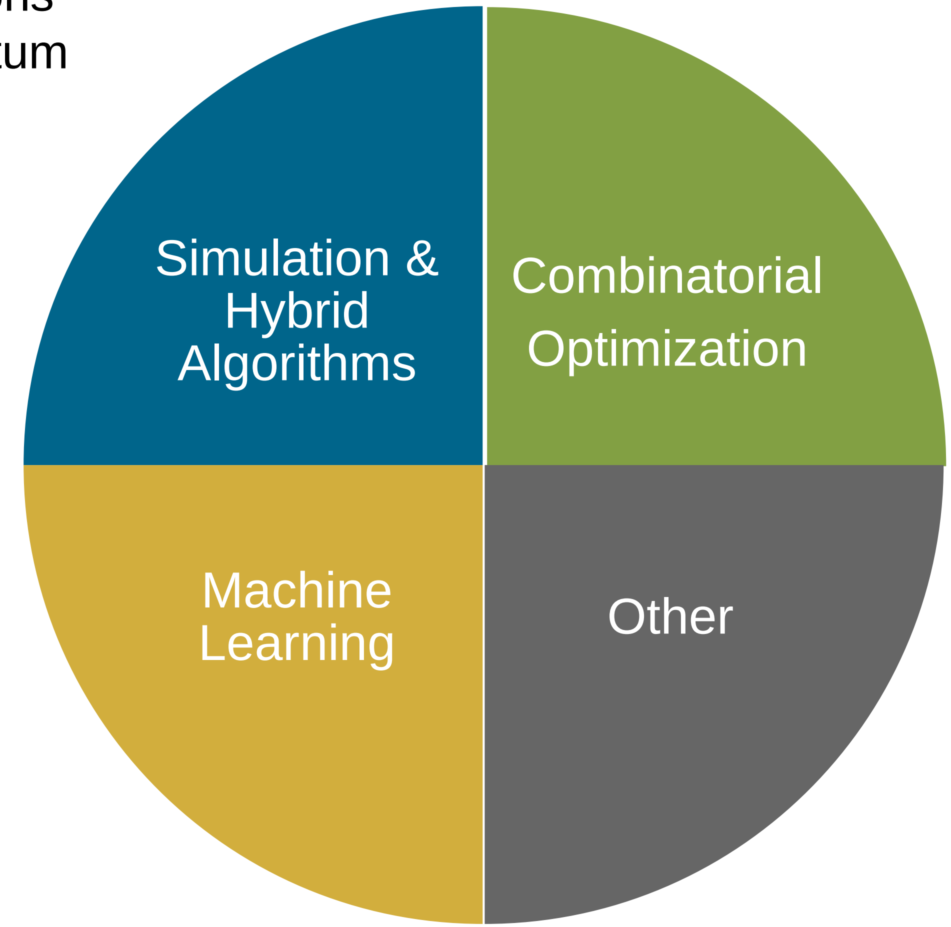
- Fauseweh, Benedikt (2023) *Quantum many-body simulations on digital quantum computers: state-of-the-art and future challenges*. **Nature Communications**. Invited review.
- Basermann, Achim und Epping, Michael und Fauseweh, Benedikt und Felderer, Michael und Lobe, Elisabeth und Schmiedinghoff, Gary und Schuhmacher, Peter und Weinert, Alexander und Wied, Yoshinta E. Setyawati (2023) *Quantum Software Ecosystem Design*. Buchkapitel.
- Carbonelli, Cecilia und Felderer, Michael und Jung, Matthias und Lobe, Elisabeth und Lochau, Malte und Luber, Sebastian und Mauerer, Wolfgang und Ramler, Rudolf und Schaefer, Ina und Schroth, Christoph (2023) *Challenges for Quantum Software Engineering: An Industrial Application Scenario Perspective*. Buchkapitel.
- Jung, Mathias und Krumke, Sven O. und Schroth, Christoph und Lobe, Elisabeth und Mauerer, Wolfgang (2023) *QCEDA: Using Quantum Computers for EDA*.



SELECTED QC APPLICATIONS

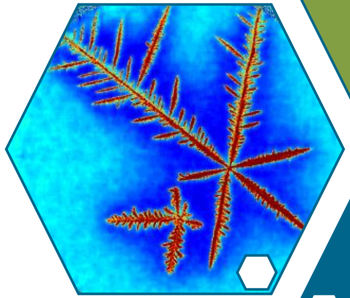
Approaches to Quantum Computing

We categorize our applications by the most promising quantum algorithmic approaches…



Subject Areas

… and the subject domain.

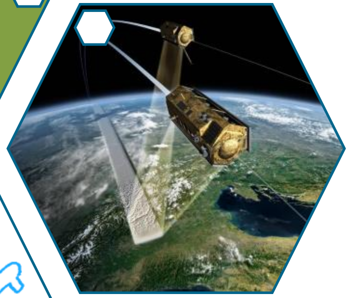


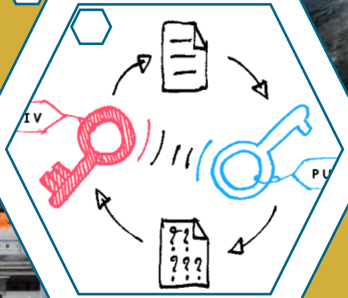
Energy systems

Logistics

Cryptography

Radar Technology



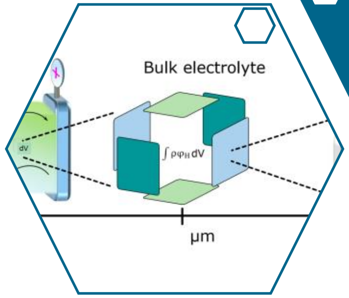


Material simulation

Battery research

Climate research

Aerodynamics



Quantum Simulation

Examples

Vibronic Structure and Dynamics

- Interaction of Electrons and molecular vibrations is called vibronics
- Often ignored in chemistry due to limited resources
- Important for quantum sensors, but also for gates and decoherence in quantum computers
- Quantum computers can simulate the interaction

Atomistic simulation of engineering alloys

- How can quantum computers enable fast & accurate material simulations?
- quantum-classical hybrid methods exploit small quantum computers
- Embedding theories split large quantum simulations into small subsystems (e.g. dynamic mean field theory)
- Simulated titanium oxide

Electron transfer in organic photovoltaics

- Follow-up project for vibronic structure and dynamics
- Use IBM Computer in Ehningen
- Simulate process of charge separation
- Use noise to emulate complex environments
- Goal: develop new design principles for solar panels

- We (as others) consider quantum simulation very promising in the near future
- Simulation of material properties is very important to many institutes of the DLR

Quantum Machine Learning

Examples

Quantum State Compression of Hyperspectral Data	Uncertainty in the calculation of glacial ice mass balances	System modelling in solar energy research
• Analysis of remote sensing data using AI • QML algorithms provide speed-up, but loading is bottleneck • States can be compressed, e.g. by compressing MPS bond dimension	• Neural networks (NNs) are used for evaluating satellite images • Estimation of the uncertainty is important • Comparison of the uncertainty for classical and quantum NNs	• Supervision of solar power plants requires quick analysis of data • Investigate whether quantum machine learning can potentially help in the future

- Many researchers already use machine learning to analyze data
- They want to know if quantum computing can improve the analysis speed or accuracy

Combinatorial Optimization

Examples

Transmission Expansion Problem	Multi-robotic fibre composite lightweight construction	Loading optimisation for autoclave processes
• Which new power plants, cables, electrolyzers should be build? • Mixed-Integer linear program (MILP), which is hard to solve • Investigate coupling classical and quantum solvers	• Optimize time schedule in a factory for leightweight construction with multiple robots • Make process faster, more versatile, and/or more robust • Formulate optimization problem for quantum annealer	• Autoclaves are airtight vessels, which are used for hardening of structures in manufacturing • Loading multiple structures into each autoclave improves time efficiency • This is a hard combinatorial optimization problem, for which quantum annealers may find better solutions

- Many combinatorial optimization problems can be mapped to the same general formulation (e.g. QUBO)
- Even medium size instances cannot be solved optimally on classical computer

Other algorithms

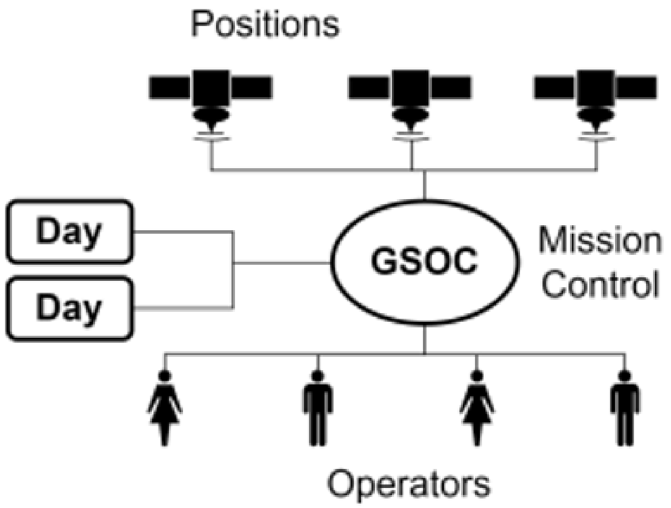
Examples

Ground motion estimation	Krylov space method	Quantum state generation with photonic quantum computers
• Use satellite-based radar interferometry to precisely observe motion of e.g. buildings • A key component of the algorithm is the multiplication of a vector with a unitary matrix → can be implemented via quantum gates	• Given a matrix A and a vector q • Space spanned by $\{q, Aq, \ldots A^{j-1}\}$ grows until j=r, the Krylow rank. • There is a maximal exponent until which the space grows, after which it is identical. • Used for solving large sparse matrices • Use parts of Shor‘s algorithm to find r	• Use a photonic quantum computer to prepare entangled N-qubit states • Analyze the achievable fidelity

- Some applications need special approaches
- Sometimes we also try to develop new quantum algorithms

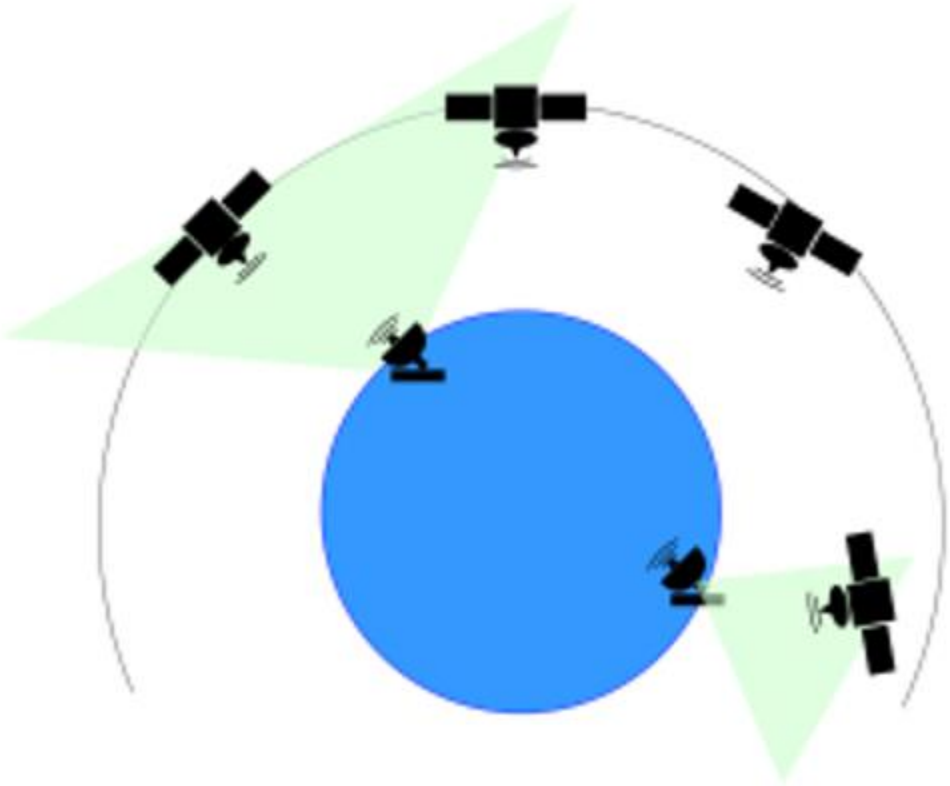
Quantum Mission Planning Challenges

- Satellites need supervision from ground control
- Assign human operators to work shifts
- Constraints:
  - Availability and skills of operators
  - Number of operators on site
  - Labour rights
- Scheduling problem, solved with Grover

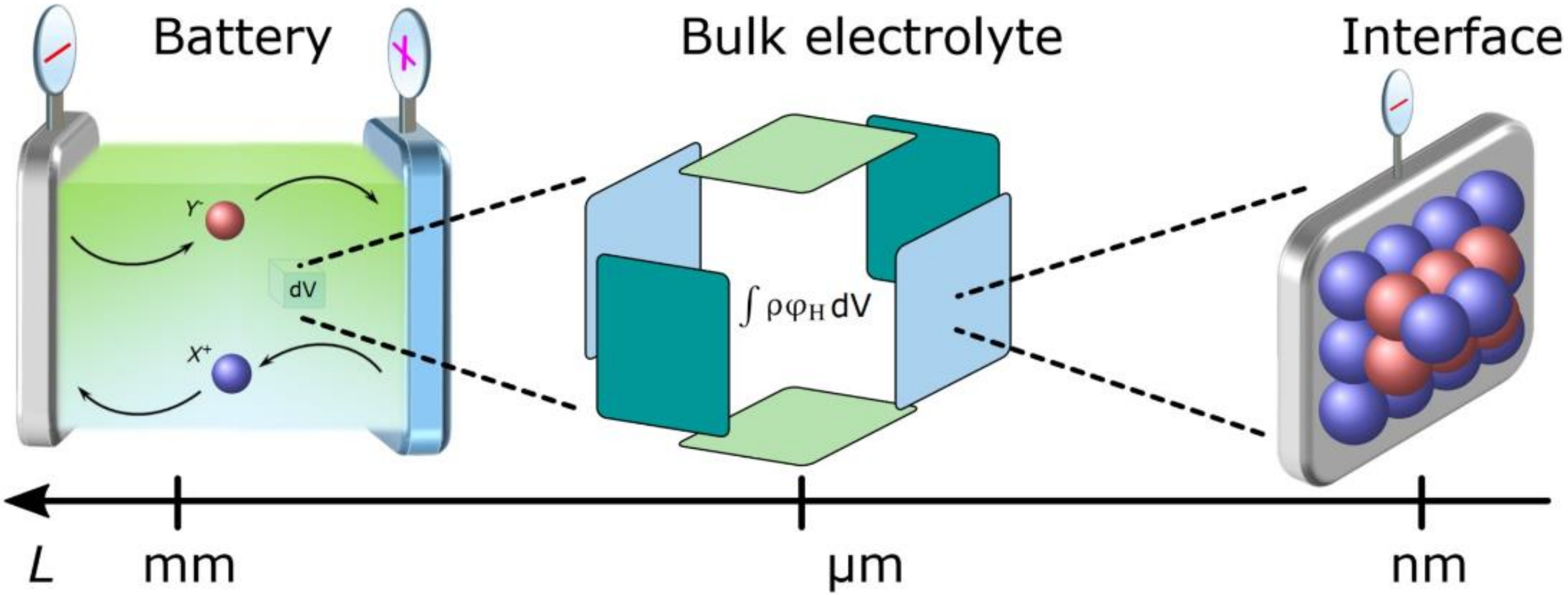


Quantum Mission Planning Challenges

- Schedule contact between satelites and ground stations
- Uniformly distribute contacts
- Constraints
  - Line of sight
  - Availability of ground station
  - Minimal and maximal distances
  - Interference

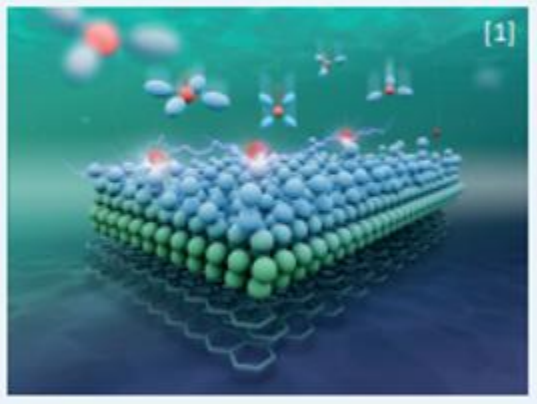


Battery material simulation

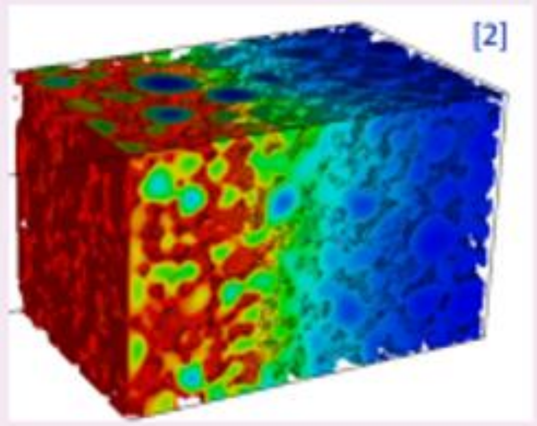


Battery material simulation

1) Material simulation
   - Scales badly clasically
   - Important for properties of electrodes, electrolytes and surfaces
   - Quantum simulation, variational quantum algorithms



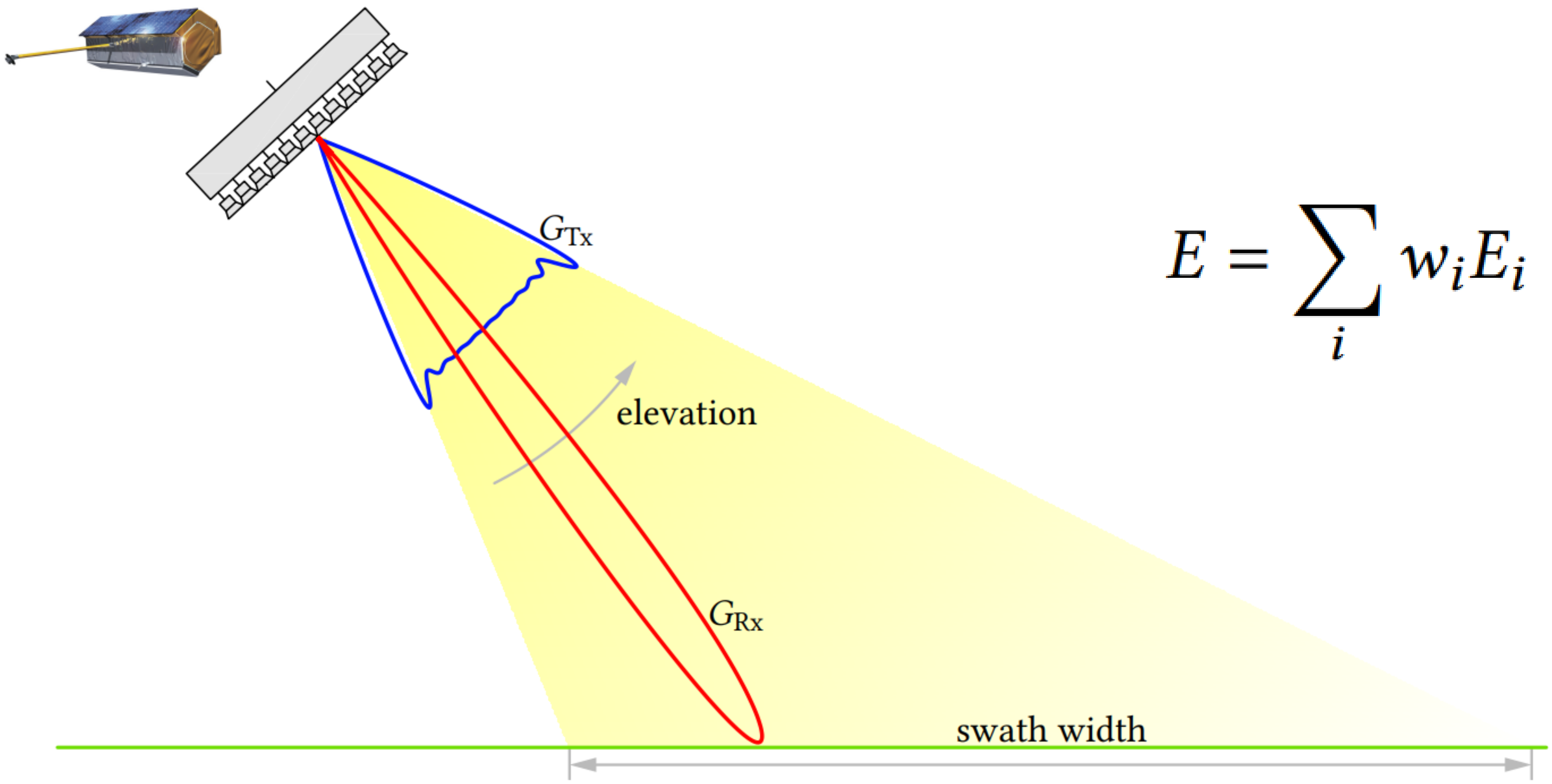
2) Partial differential equations
   - Development of numerical solvers (e.g. based on HHL)
   - Example: Diffusion equation
   - Implementation on our hardware



[1,2] For more information please see project page on qci.dlr.de

ANTENNA OPTIMIZATION

Antenna Optimization



$$E = \sum_i w_i E_i$$

- **Given:** Array of antennas with known radiated fields E_i
- **Goal:** Find weights w_i so the total power $|E|^2$ matches a target pattern as good as possible

Optimization Goals

a) Feasibility with constraints of the form:

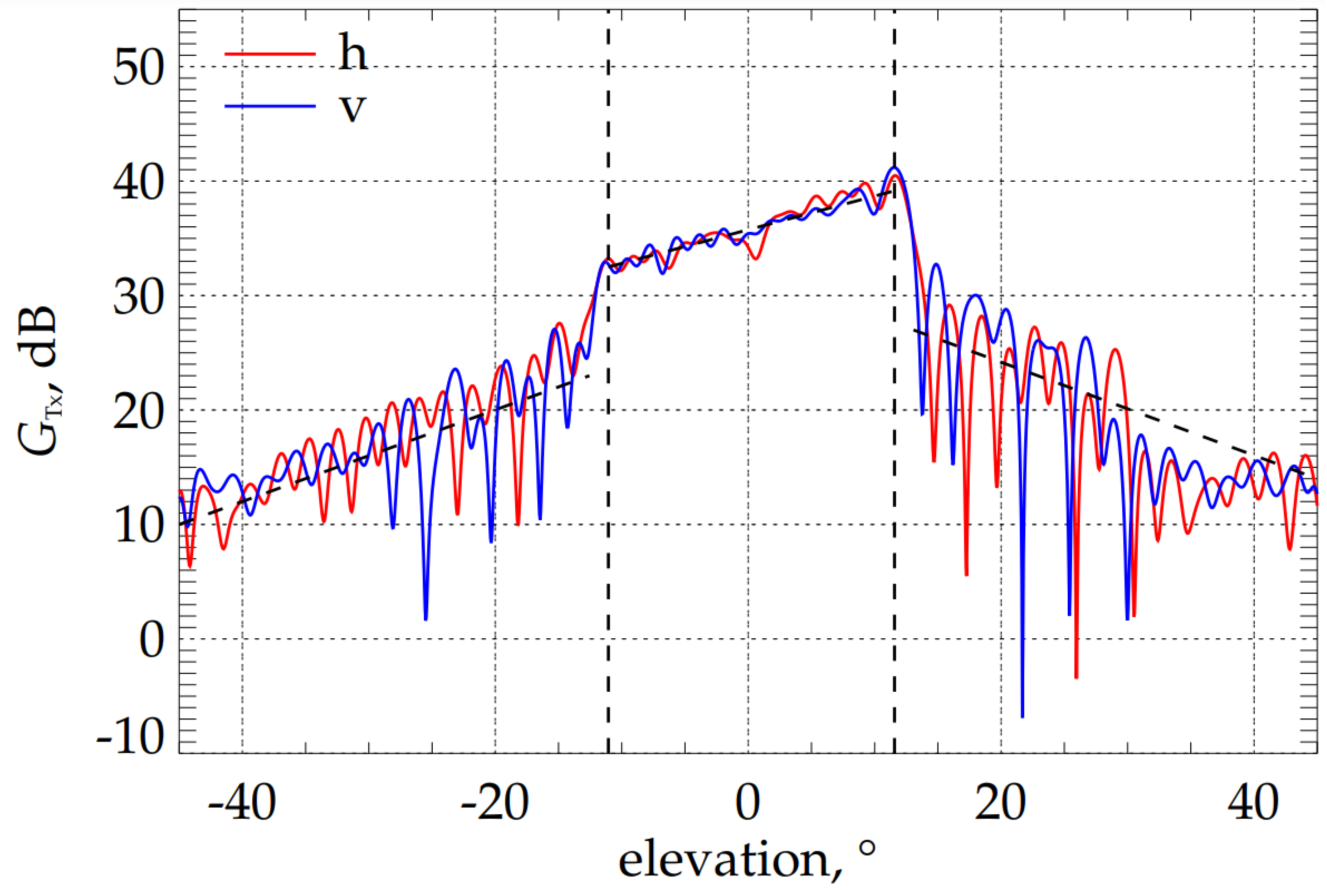
$$G(\vartheta_l) \geq \tilde{G}(\vartheta_l)$$

$$G(\vartheta_m) \leq \tilde{G}(\vartheta_m)$$

b) Minimize pattern mismatch:

$$\text{minimize} \quad \sum_{lm} \left(G - \tilde{G}\right)^2 (\vartheta_{lm}) \,,$$

$$\text{subject to} \quad |w_i| = 1 \quad \forall\, i \,.$$



For us gain G_{Tx} and power $|E|^2$ are the same up to a constant factor

Using a quantum annealer

- Split numbers into real and imaginary part
- Encode both in binary representation, e.g.

$$w_n^{\mathcal{R}/\mathcal{I}} = \frac{1}{2^K} \sum_{k=0}^{K} 2^k x_{nk}^{\mathcal{R}/\mathcal{I}} - 1$$

- Objective now a binary polynomial of degree 4.
- Our software library QUARK[1]
  - introduces slack variables to make it degree two
  - adds penalty terms for the constraints
  - runs the QUBO (quadratic unconstrained binary optimization), e.g. on D-WAVE annealer

Image: FZ Jülich

[1] gitlab.com/quantum-computing-software/quark

Interference Simulation

- Use amplitude encoding to represent the fields E_i and weights w_j:

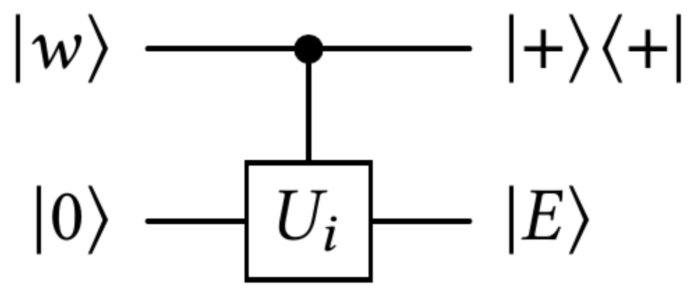
$$|w\rangle = \sum_j w_j \, |j\rangle \qquad |E_i\rangle = \sum_j E_i(\theta_j)\, |j\rangle$$

- Let U_i prepare $|E_i\rangle$, i.e. $U_i\,|0\rangle = |E_i\rangle$.
  Construct a controlled operation

$$U = \sum_i |i\rangle\langle i| \otimes U_i$$

- Then:

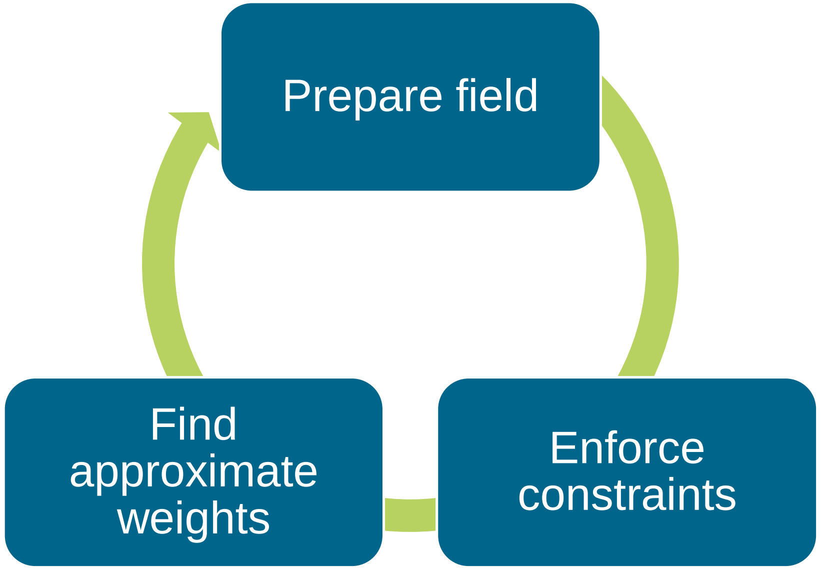
$$\langle +|\, U \,|w\rangle\, |0\rangle = \langle +| \sum_i w_i \,|i\rangle\, |E_i\rangle \propto \sum_i w_i \,|E_i\rangle = |E\rangle$$

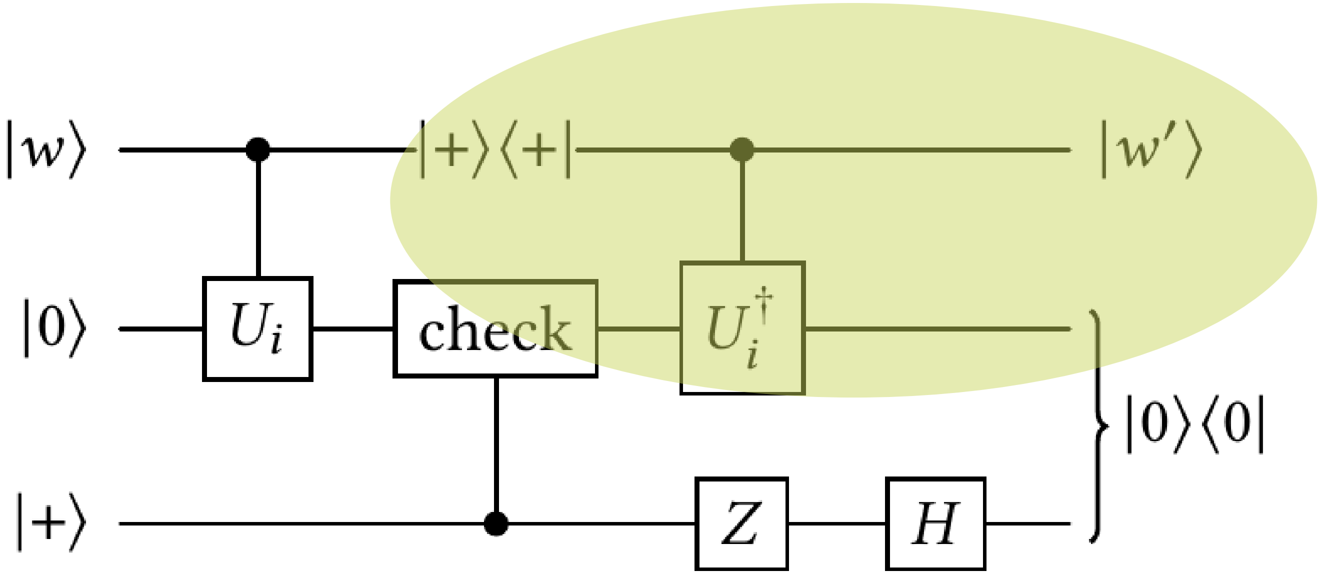


A gadget to superpose the fields using post-selection.

Interference Simulation: Field inversion approach

- Invert circuit to map field to weights
- Iterative approach:





Interference Simulation: Field inversion approach

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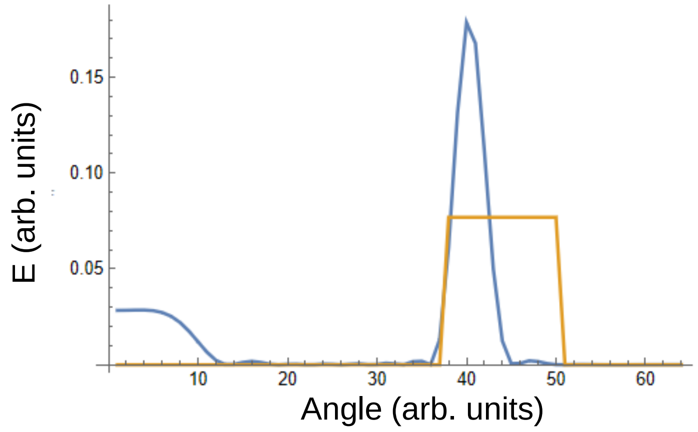
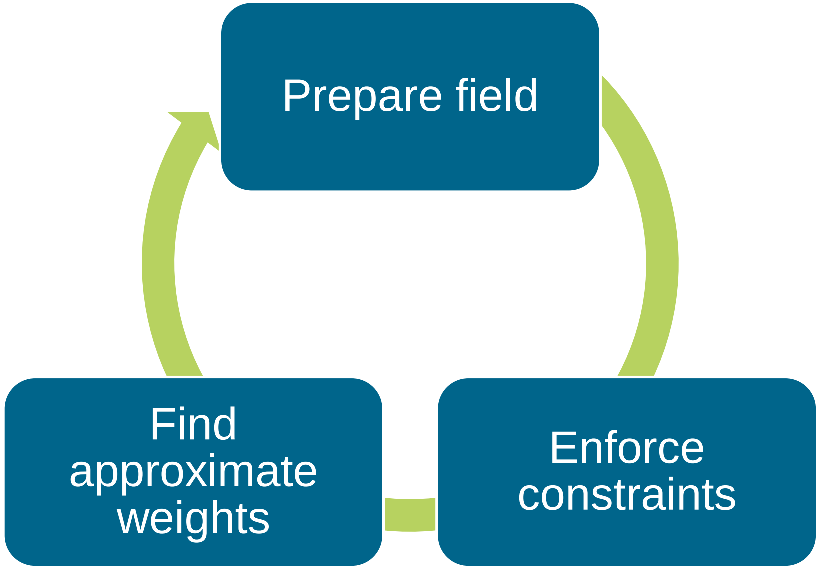
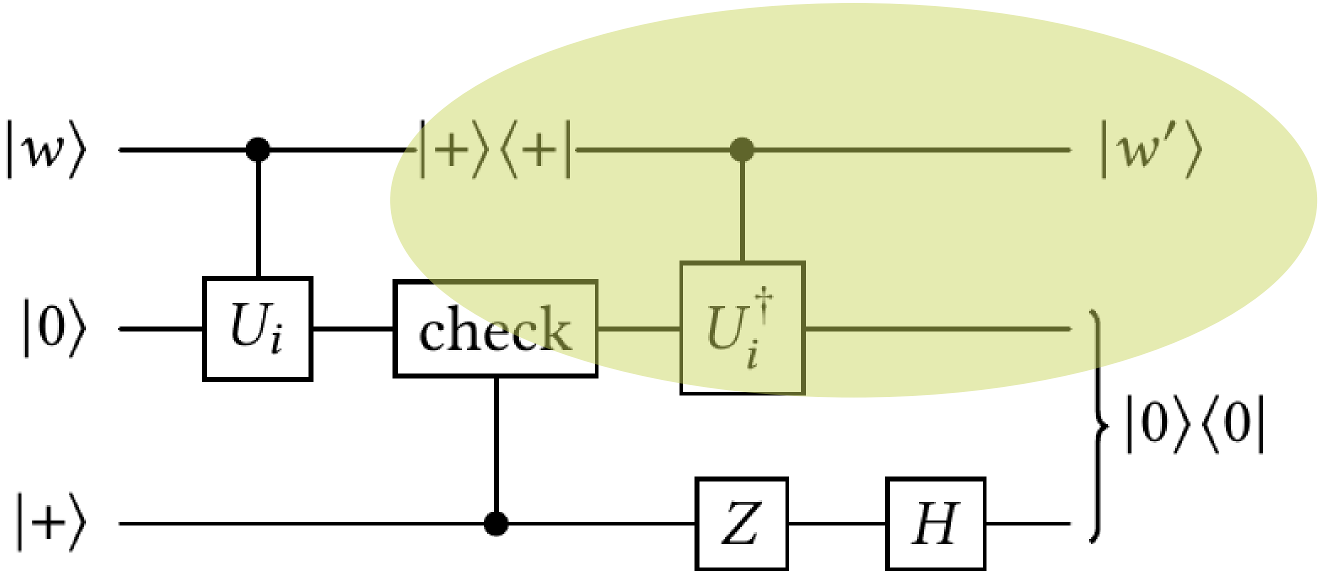






Interference Simulation: Hybrid antenna optimization

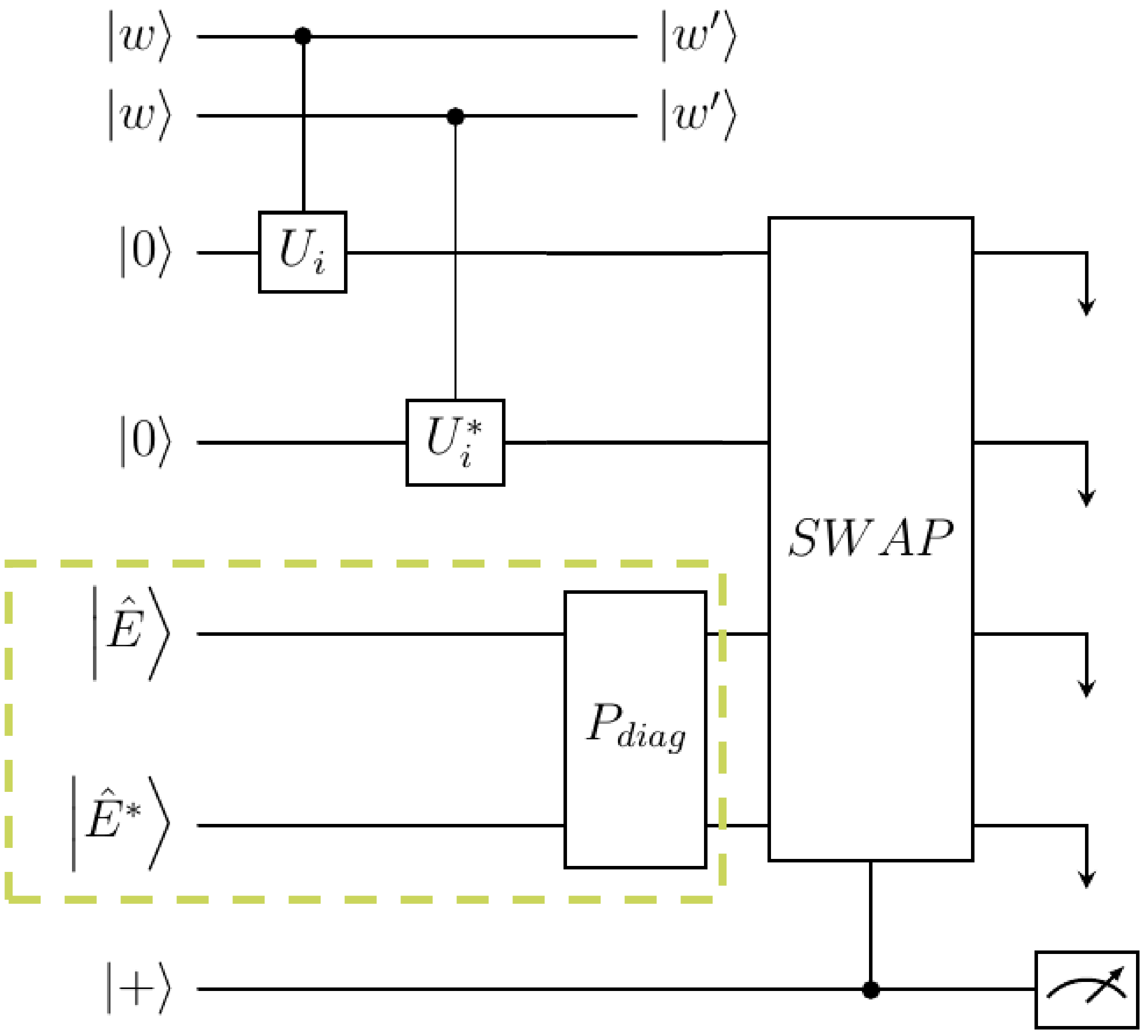
- Use SWAP test to measure similarity of produced pattern and target pattern

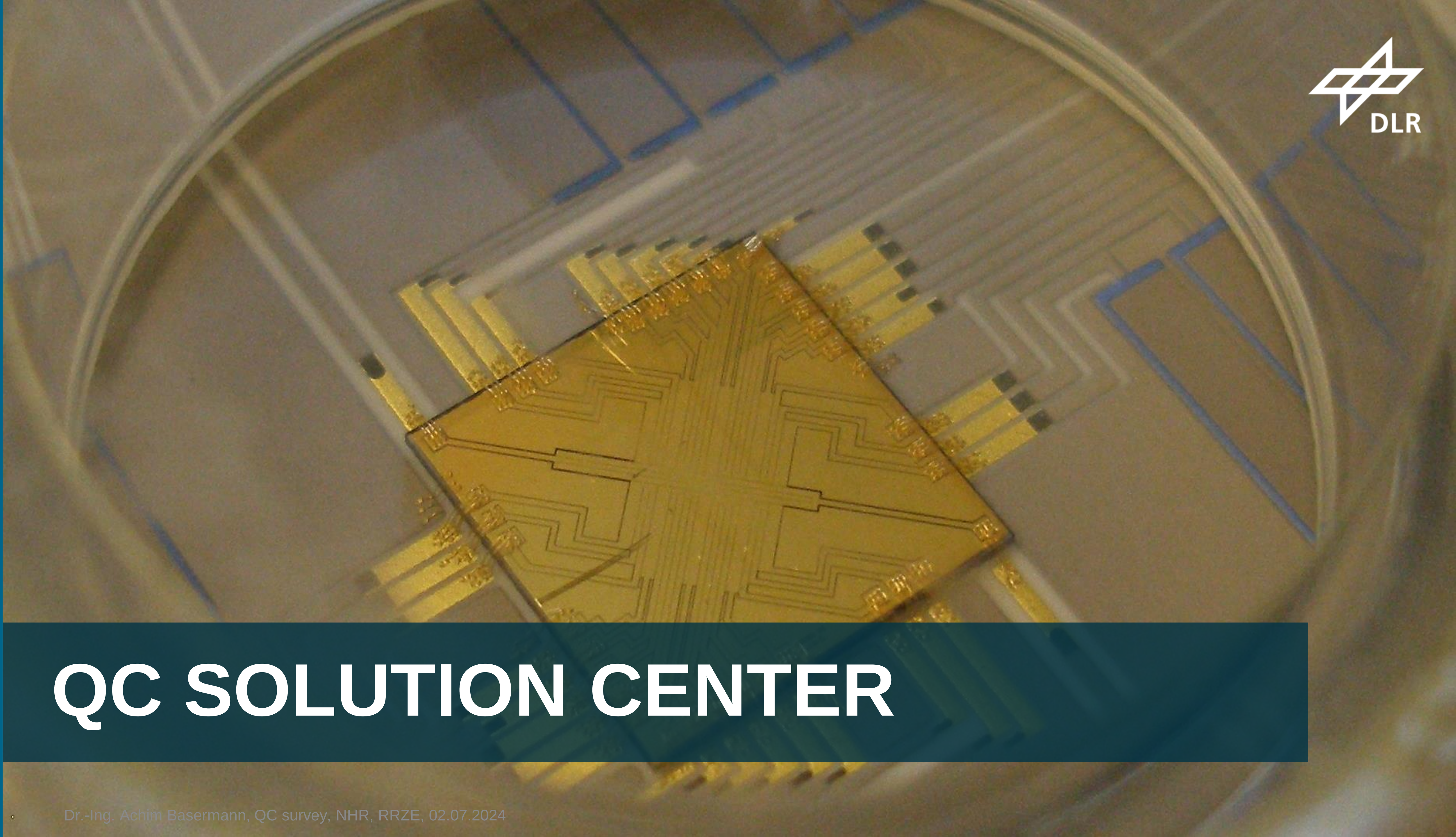
$$P(0) = \frac{1}{2} + \frac{1}{2} |\langle\psi|\phi\rangle|^2$$

- Additional trick:
  Squared amplitudes are contained in the product state

$$|E_i|^2 = \langle ii| \, |E\rangle \, |E^*\rangle$$

- Optimize in classical outer loop





QC SOLUTION CENTER

Concept

- In Hamburg, DLR is developing a unique, **complete QC stack** and has **access** to an extensive portfolio of **quantum computers**
- DLR's QC Solution Center offers a comprehensive portfolio of **services for companies** and organisations for QC solutions in different application domains

Purpose of the QC Solution Center

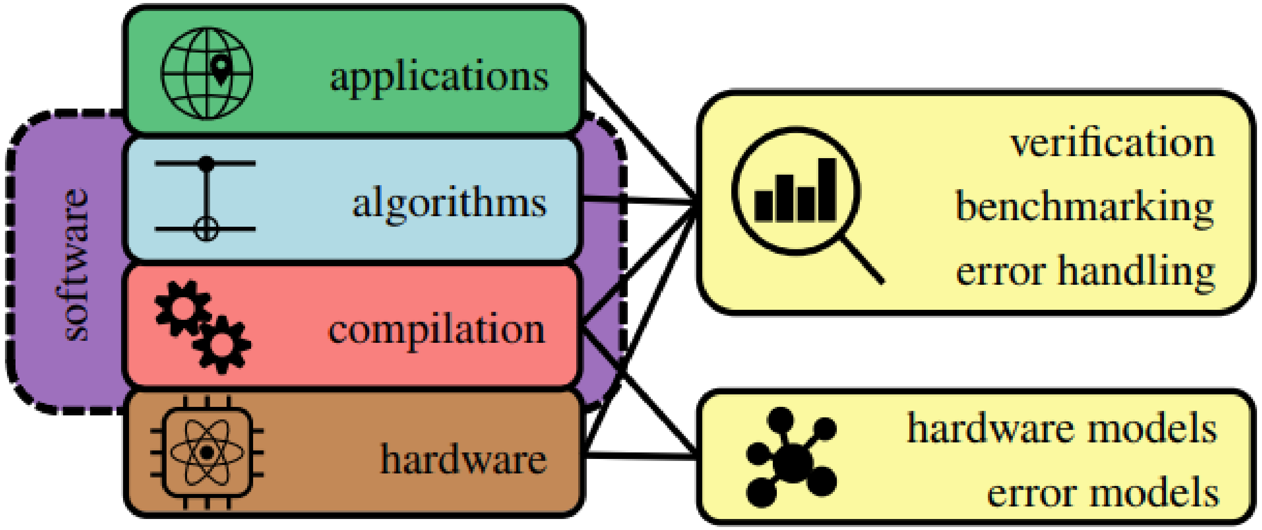
- Services of the QC Solution Centre
  - Analysis of industrial use cases & concept studies
  - Creation of algorithms and joint testing on DLR quantum computers
  - Benchmarking of different platforms and the respective use case
  - Training and education
- Possible areas of application (examples)
  - Combinatorial optimisation (planning problems), quantum simulation
  - Artificial intelligence, cryptography

Concept Studies

- Duration 6 months
- Jointly between industry partner & DLR QC Solution Centre
- Exemplary process:
  1. Appointment of industrial contacts and definition of the use case
  2. Joint kick-off at DLR in Hamburg
  3. Presentation of the use case & data structure
  4. Assessment of mathematical suitability for QC
  5. Modelling of the problem and implementation of the algorithms on simulator or quantum computer(s)
  6. Preparation of final report for industrial partners

Technical Features

- Access and therefore adaptability at all levels of the QC stack
- Suitable abstraction layers
- Solution patterns
- Hybrid computing
- Integration of SW/HW manufacturer and user



Many thanks for your attention!

Department Head: Dr.-Ing. Achim Basermann

Vice Department Head: Dr. Alexander Rüttgers

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http://www.DLR.de/sc