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Fraunhofer Institute for Integrated Systems and Device Technology IISB

Simulation for (and with) Quantum Computers

Georg Kruse, Simon Mundinar – 12.10.2023 – IISB Annual Symposium 2023

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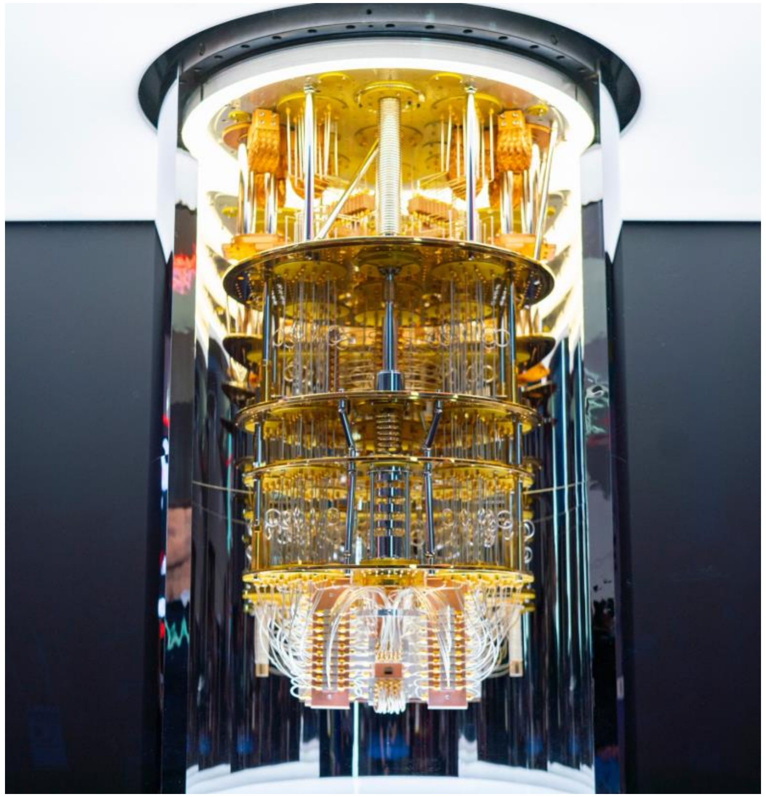

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Part 01

Quantum Computer

Quantum Computer

Qubits: Physical System

General Properties

- Any quantum 2-state system can act as a qubit
- However, for useful qubit **additional properties** are necessary:

- **Long relaxation and decoherence times**
  - Lifespan of the qubit's state (e.g., superconducting qubits ~100 µs; trapped-ion qubits ~10 min)

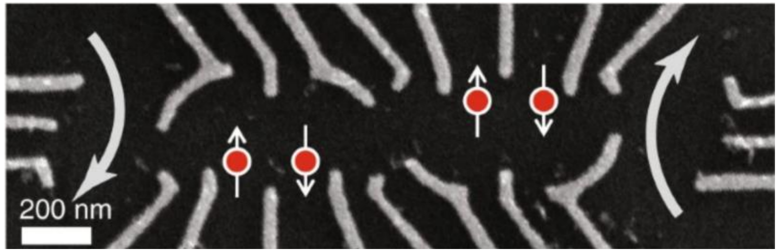
- **Scalable**
  - One qubit not enough for computing, required are hundreds and more (record: 433 qubits)

- **Controllable**
  - Qubits need to be manipulated and read out, otherwise we cannot do anything

- **Efficiently manufacturable**
  - Ideally no variation between qubits (and cheap production)

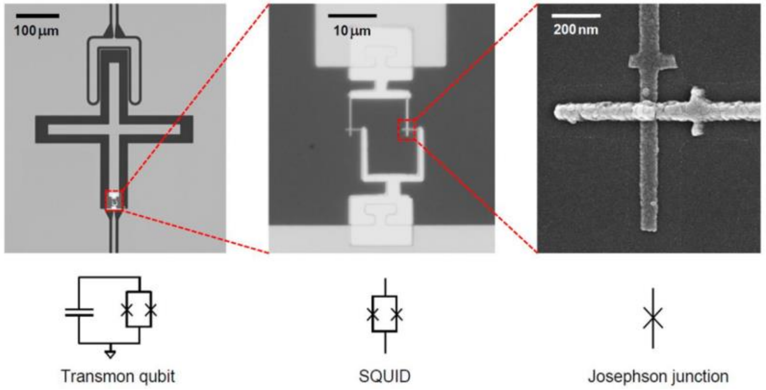
Qubit Architectures

- Huge number of different architectures possible, e.g., color centers, double quantum dots, superconducting circuits, trapped ions, trapped atoms, etc.



2 double quantum dot qubits

J. M. Nichol, *et al.*, npj Quantum Information **3**, 3 (2017)



Superconducting Transmon qubit

T. E. Roth, *et al.*, arXiv:2106.11352 (2021)

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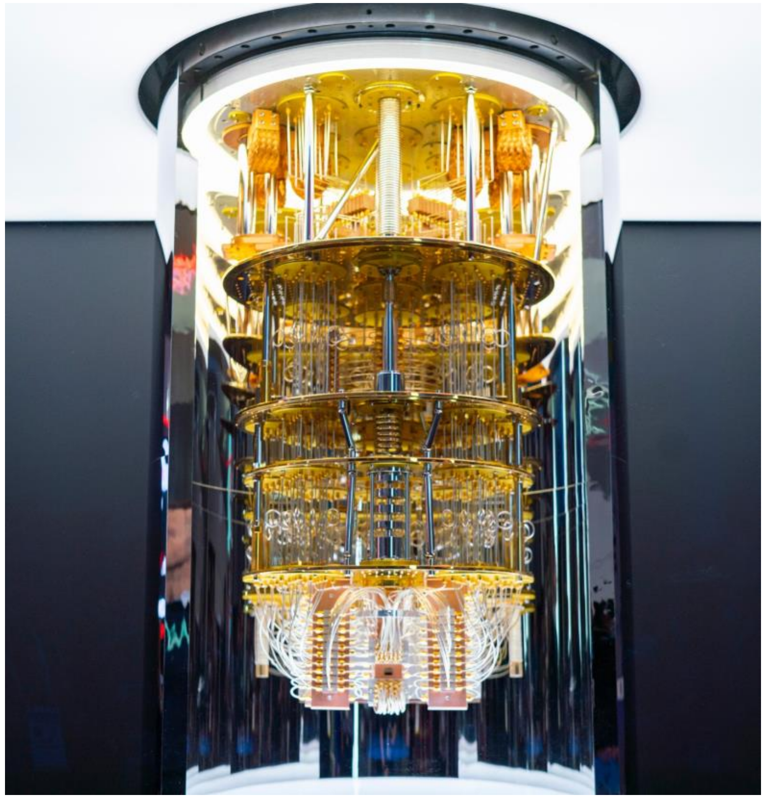
Quantum Computer

Some Manufacturers



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Quantum Computer

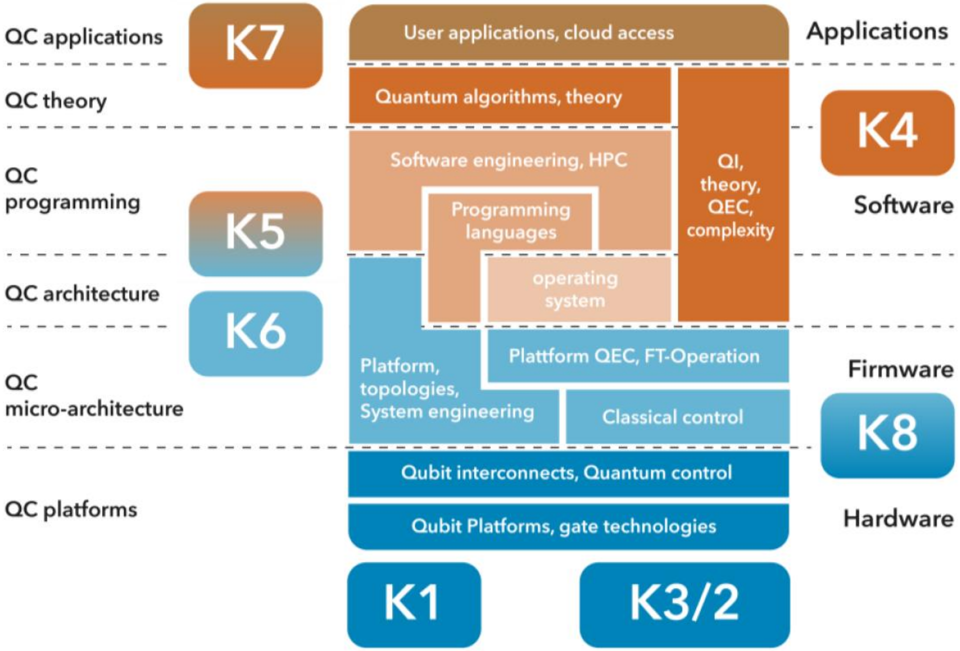
Munich Quantum Valley

Munich Quantum Valley

Building a Bavarian Quantum Computer

- Large Bavarian research project 10/2021 – 09/2026
- From qubit research through integration and application to education

- IISB contributes to consortia
  - K6 "Scalable Hardware & Systems Engineering" (SHARE)
  - K7 "Quantum Algorithms for Application, Cloud & Industry" (QACI)



BAdW Bayerische Akademie der Wissenschaften | Fraunhofer | Max Planck Gesellschaft
DLR Deutsches Zentrum für Luft- und Raumfahrt | FAU Friedrich-Alexander-Universität Erlangen-Nürnberg | LMU Ludwig-Maximilians-Universität München | Technische Universität München TUM

Part 02

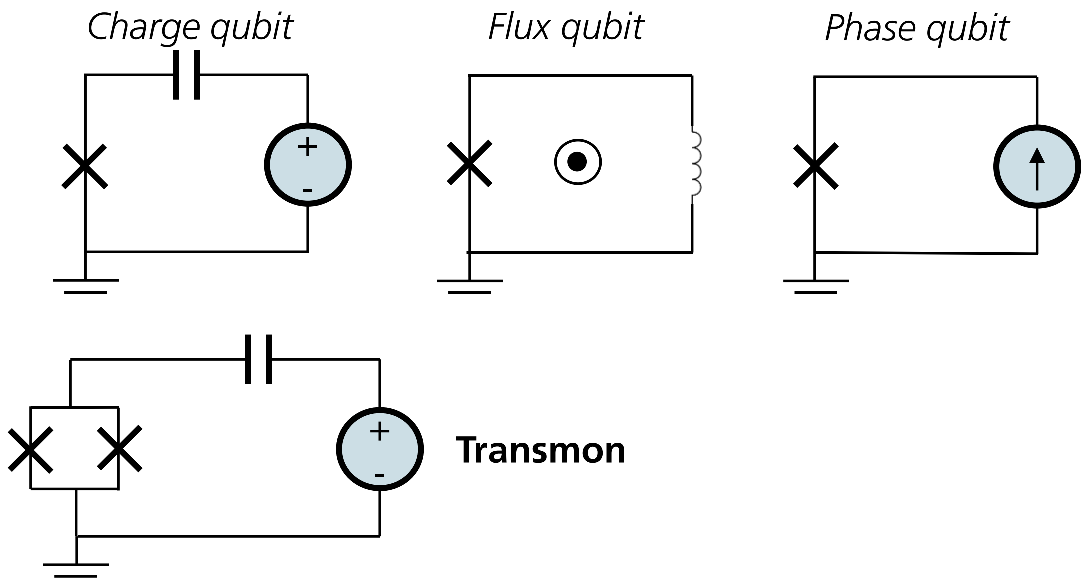
Simulation for Quantum Computers

Simulation for Quantum Computers

Superconducting Qubits

Architectures

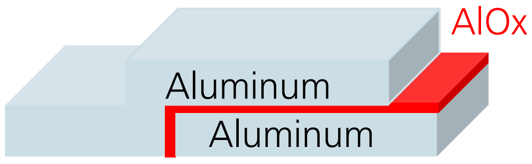
- Several different architectures of superconducting qubits



- Very different physics for different architectures
- All of them based on Josephson junctions

Josephson junctions

- Superconductor-Insulator-Superconductor junctions
- Since superconductors are required, cryogenic temperatures are essential (usually ~ mK)
- **Josephson effect**: Supercurrent through the junction without external voltage



- Electrical transport based on tunneling effect
- Acts as nonlinear inductance, leading to anharmonicity in the oscillator circuits that are the qubits

- Several tasks identified which need simulation support
  - Here 2 examples

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Simulation for Quantum Computers

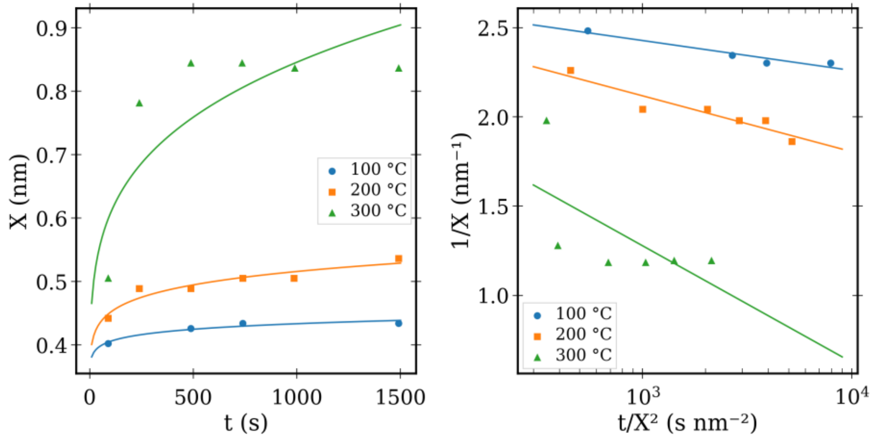
Simulations for Josephson Junctions

Aluminum oxidation

- **Questions**: How does Aluminum oxidize? Are their possibilities to improve the oxidation process?
- Simple model: **Cabrera-Mott theory** with corrections by Ghez [1,2]

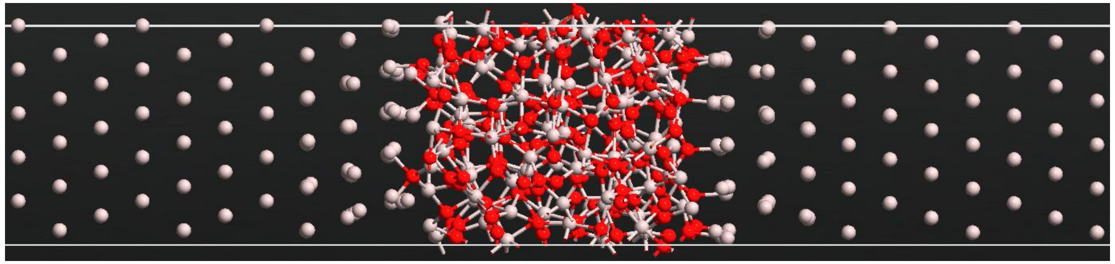
$$\frac{\mathrm{d}X}{\mathrm{d}t} = 2u \sinh\left(\frac{X_1}{X}\right), \text{solved by } \frac{1}{X} = -\frac{1}{X_1}\left(\ln\frac{t}{X^2} + \ln X_1 u\right)$$

- **Calibration** based on experimental data from Jeurgens [3]

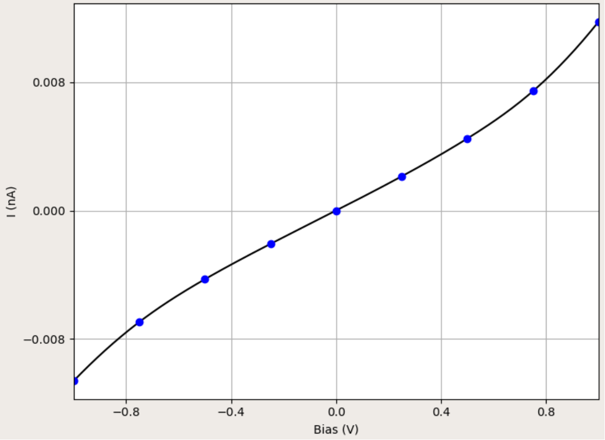


Impact of the oxide

- **Question**: What is the impact of the oxide properties on the current?



- Create oxide with **Molecular Dynamics**
- I(V) curve calculated using **Nonequilibrium Green's Functions** Method
- Differences in the I(V) curve due to oxide stoichiometry
- Also differences due to oxide thickness



[1] N. Cabrera and N. F. Mott, Rep. Prog. Phys. **12**, 163 (1949) [2] R. Ghez, J. Chem. Phys. **58**, 1838 (1973) [3] L. P. H. Jeurgens, *et al.*, J. Appl. Phys. **92**, 1649 (2002)

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Simulation for Quantum Computers

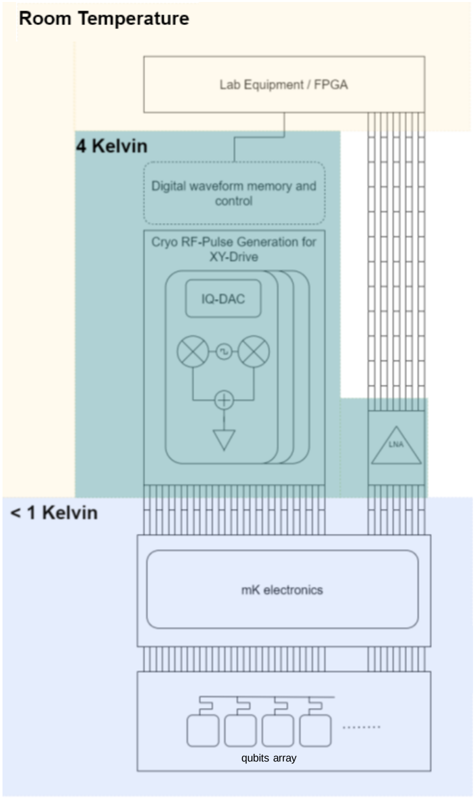
Control Electronics

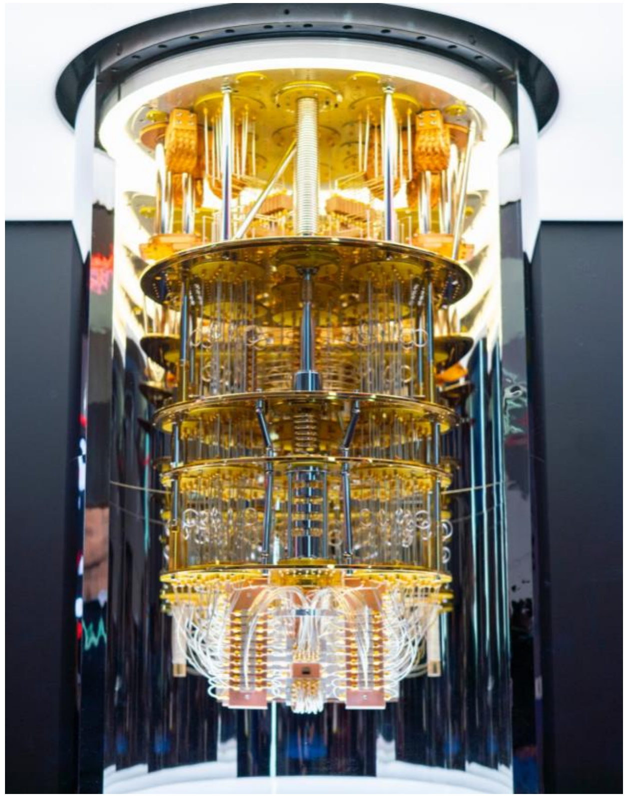
Controller and Read-out

- Qubits need to be controlled and read-out: Most convenient is electronic read-out
- Controller made in classical electronics: CMOS technology

Temperature strategies

- State-of-the-art quantum computers
  - Qubits at cryogenic temperatures
  - Controller at room temperatures
  - Not scalable system, too many cable connections
- Future quantum computers
  - Qubits and controller at cryogenic temperatures
  - More integrated systems
  - Enable large scale quantum computers





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Simulation for Quantum Computers

Control Electronics at Cryogenic Temperatures

Transistors at cryogenic temperatures

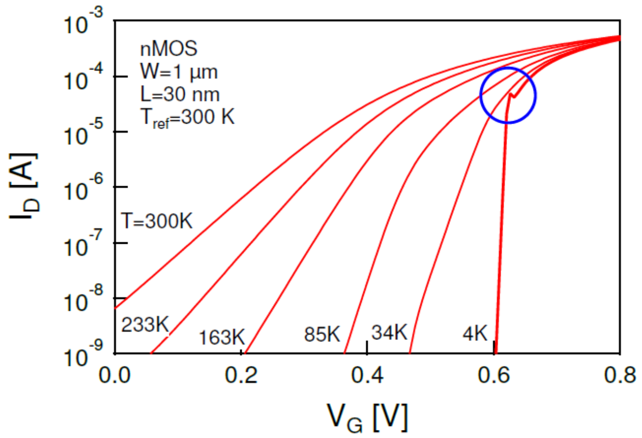
- Transistors behave differently than at room temperatures
- Current simulation models do not work and need to be adapted
- Design of controller based on simulations of individual transistors
- **Question**: How do transistors behave at cryogenic temperatures?

Measured electrical characteristics

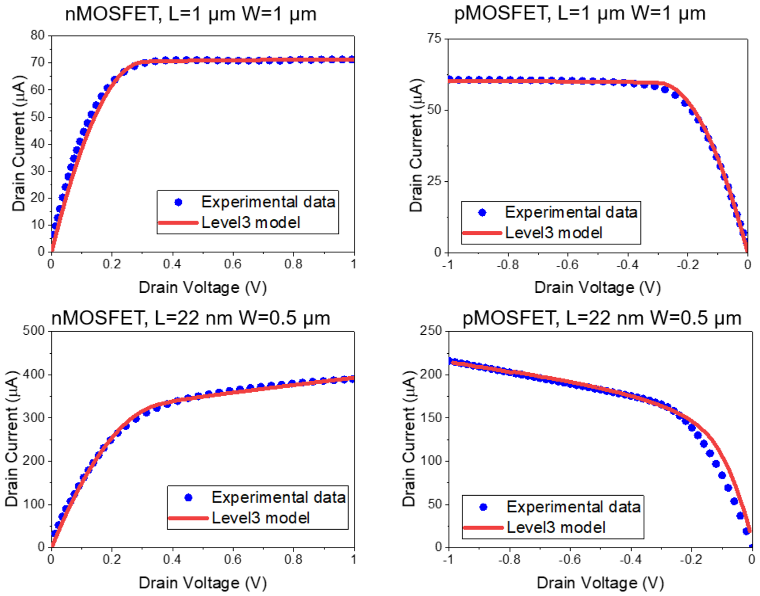
Generic compact model
describing device architecture

Model parameter extraction

Final compact model in PDK
describing a specific technology



Conventional models of 28-nm commercial bulk CMOS technology



Some results at T= 3K

Part 03

Simulation with Quantum Computers

Quantum Computing

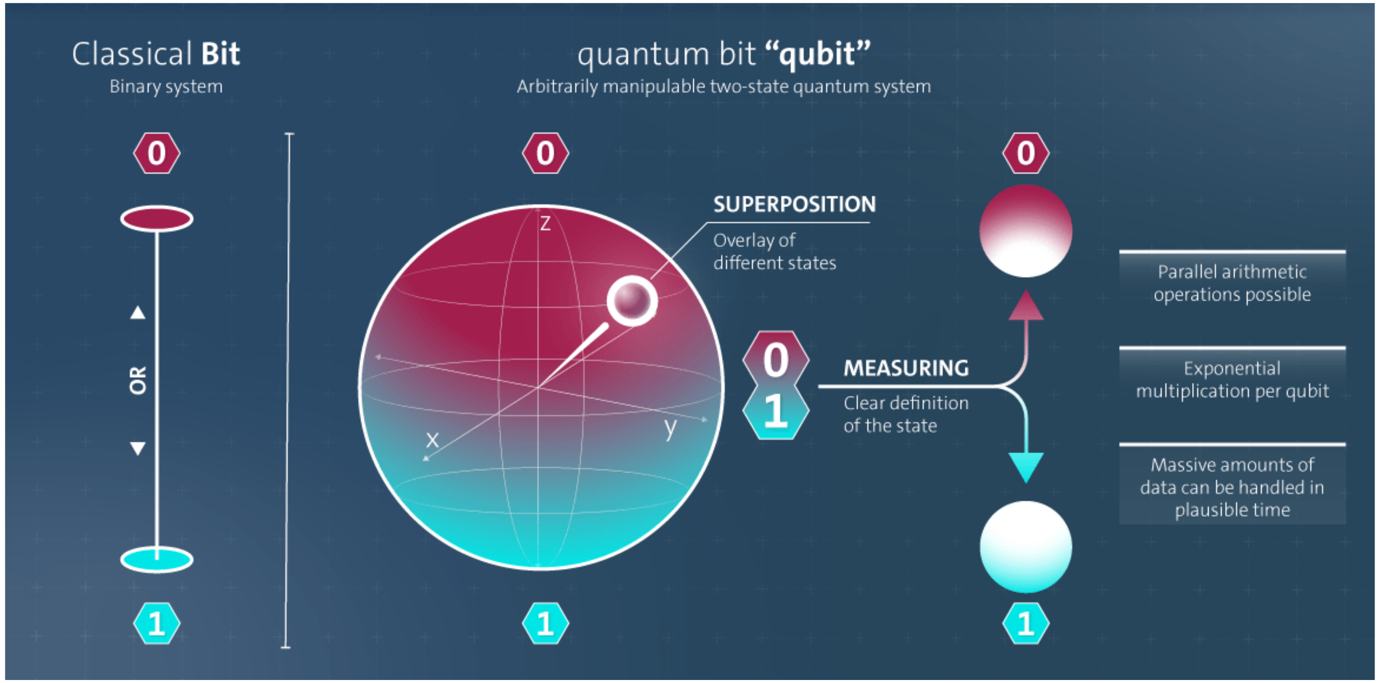
(Logical) Qubits

General Properties

- **Bit**: Classical 2-state system with discrete states (e.g., coin flip)
- **Qubit**: Quantum 2-state system (e.g., spin ½)
- **Superposition**:
  - Qubit can be in any state on Bloch sphere until measured

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

  - After measurement: $|\psi\rangle = |0\rangle$ or $|\psi\rangle = |1\rangle$ with probability α^2 and β^2
- **Entanglement**:
  - State space (“information”) scales with 2^n



Volkswagen. 2019. "Where is the Electron and How Many of Them?" Volkswagen Group. Accessed 2021-12-27.

Scaling Example

- **10 Qubits :** 2^{10} = 1,024 values
- **100 Qubits:** 2^{100} = more values than stars in the known universe

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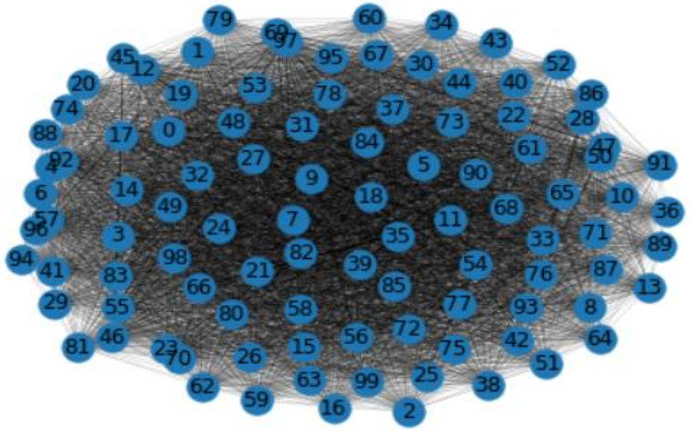
Quantum Computing

… and the Curse of Combinatorial Problems

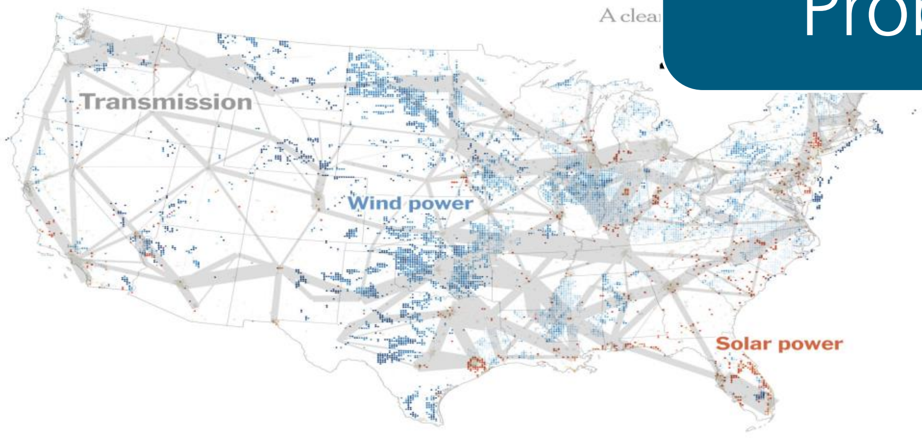
Task: Connect all nodes while minimizing the total length of the edges

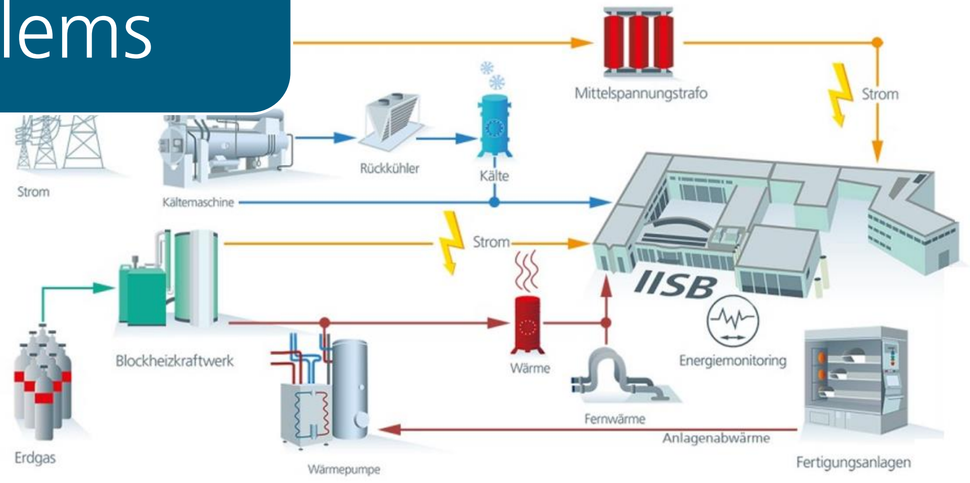


As the number of possible paths grows exponentially with the number of nodes in the graph, quantum advantage is to be expected.

Quantum Computing
Real World Applications

Combinatorial Problems





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Quantum Computing at IISB

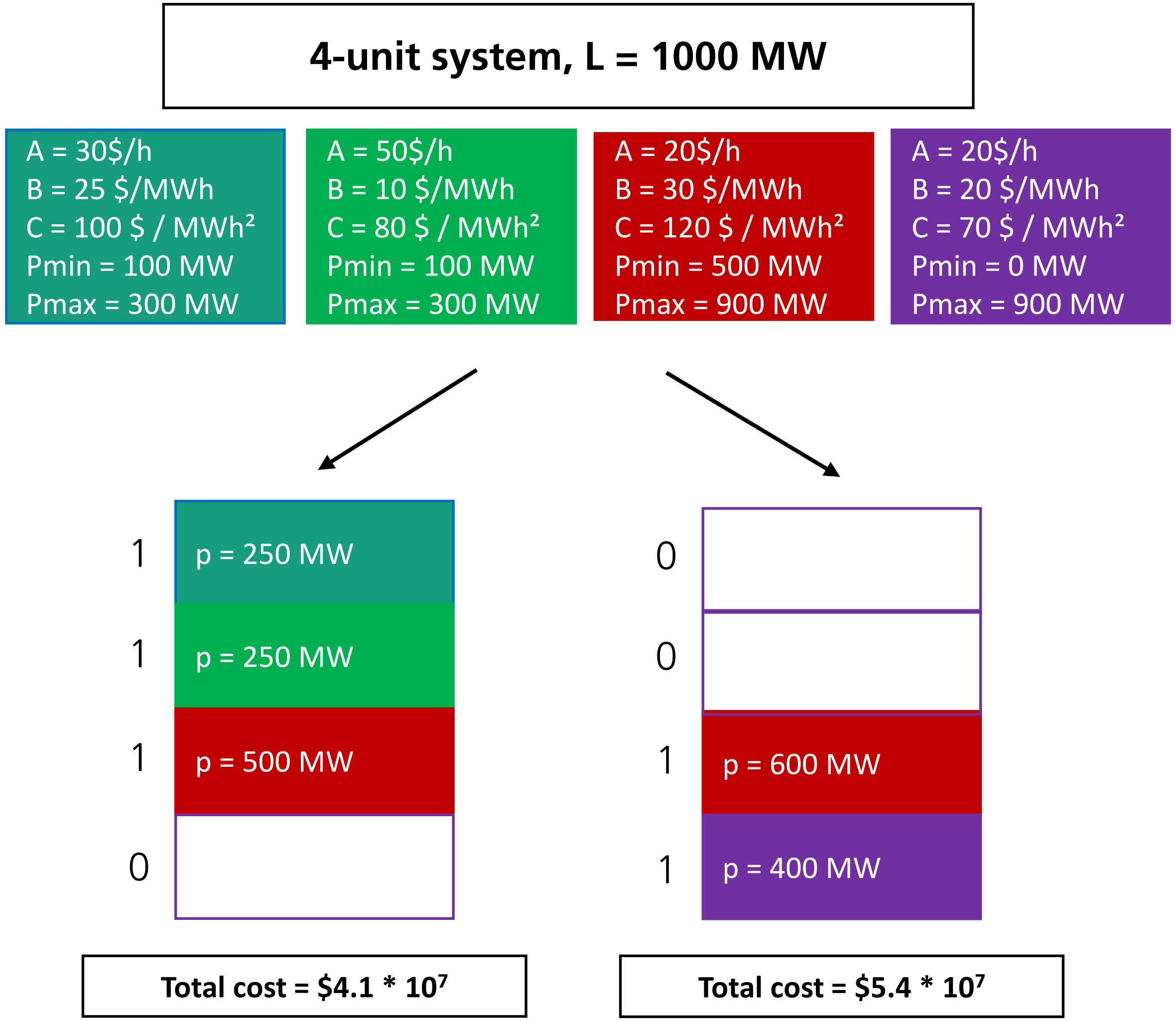
Quantum Approximate Optimization Algorithm

Unit Commitment Problem

- **Required demand needs to be met** by power plats at each timestep **while minimizing the cost of energy production**
- Mixed Integer Non-Linear Problem
- Classical Solution: MIP Solvers (CPLEX, Gurobi)

Quantum Approximate Optimization Algorithm (QAOA)

- Each **binary variable** can be encoded into one **qubit**
- Problem is encoded into quantum circuit
- Parameters of quantum circuit are optimized using classical optimizer
- QAOA is a hybrid quantum classical algorithm



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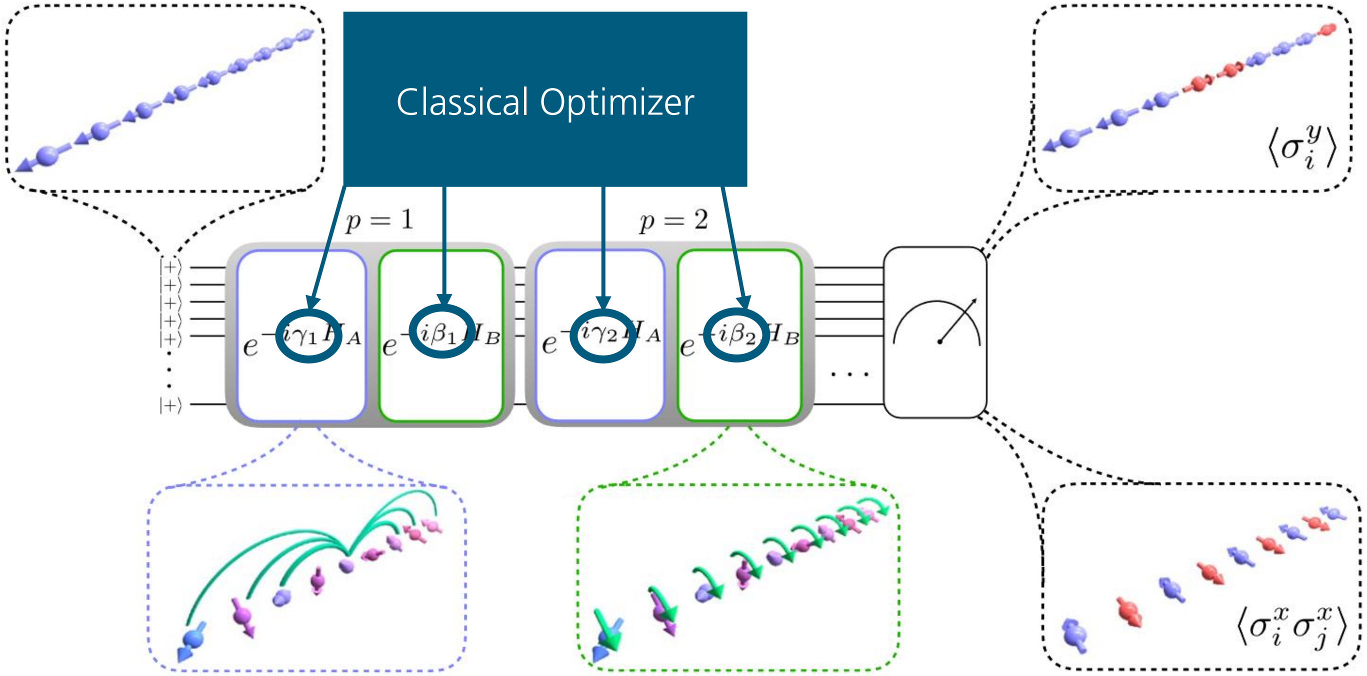
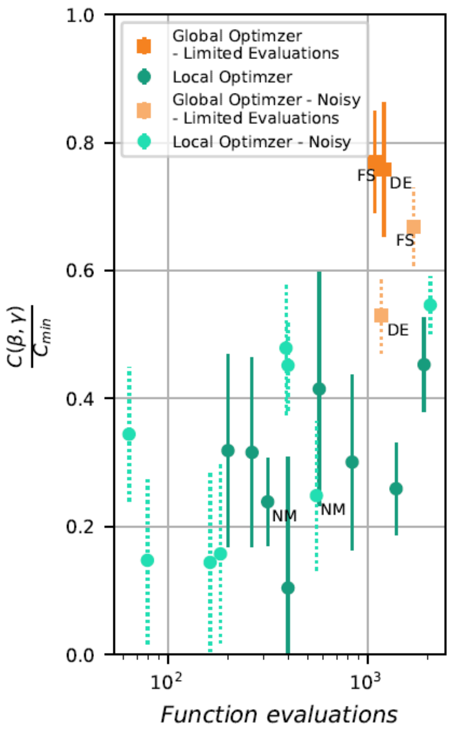
Quantum Computing at IISB

Quantum Approximate Optimization Algorithm



Pagano, Guido, et al. "Quantum approximate optimization of the long-range Ising model with a trapped-ion quantum simulator." *Proceedings of the National Academy of Sciences* 117.41 (2020): 25396-25401.



Gleißner, Peter, Georg Kruse, and Andreas Roßkopf. "Restricted Global Optimization for QAOA." *arXiv preprint arXiv:2309.12181* (2023).

State of the Art

- Access to 27 Qubit System IBM Q in Ehningen
- Evaluation of <u>classical optimizers</u> for QAOA
- Great difficulties remain **<u>qubit number</u>** and **<u>noise</u>**

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Thank you for your attention!

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