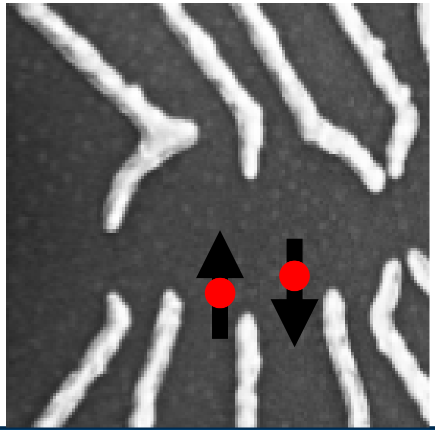

QUANTUM COMPUTER SIMULATORS / QUANTUM COMPUTER USER FACILITY JUNIQ

DATA SCIENCE AND QUANTUM COMPUTING WORKSHOP, TRIUMF, JUNE 27-29, 2018 I KRISTEL MICHIELSEN

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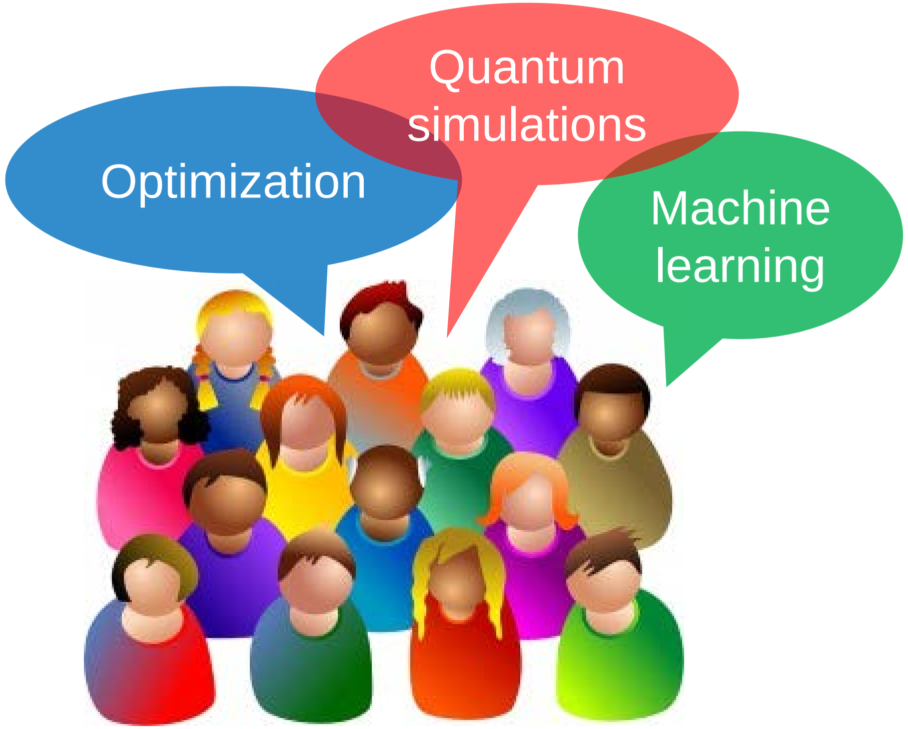
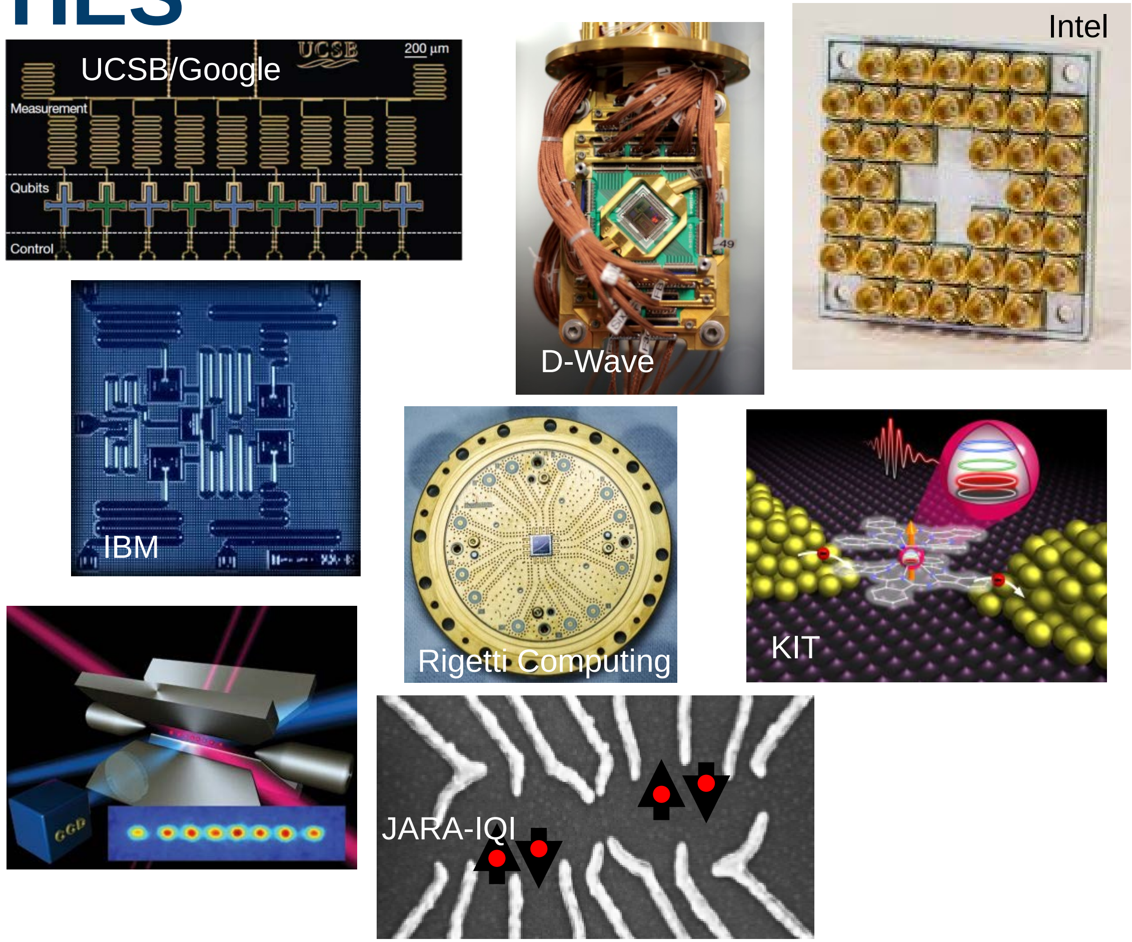
CHALLENGES AND OPPORTUNITIES

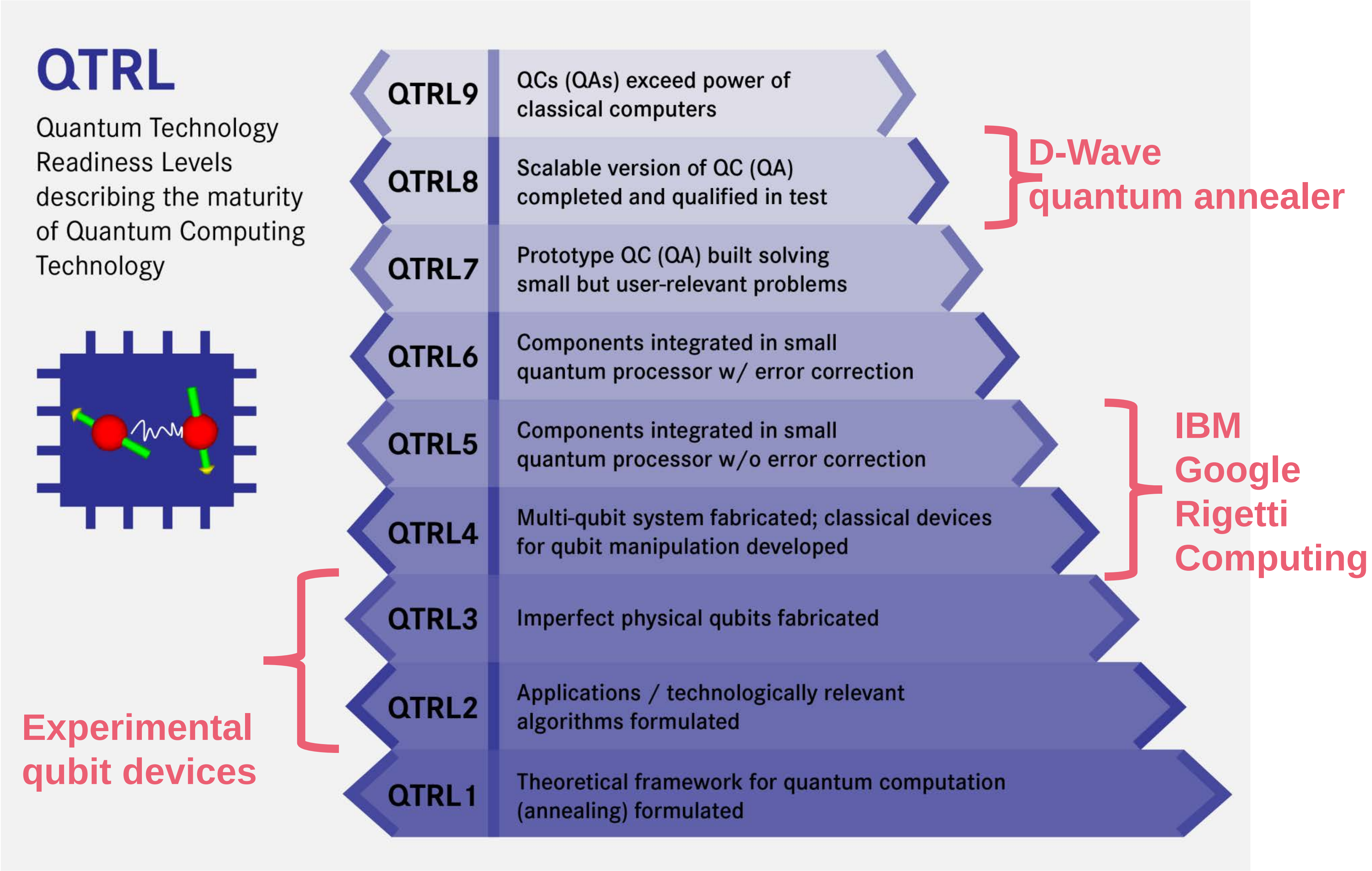


Science & Industry:
Diverse user group with various hard computational challenges



Diverse collection of qubit devices for quantum annealing and quantum computation → new computing technology

QUANTUM TECHNOLOGY READINESS LEVELS



(http://www.fz-juelich.de/ias/jsc/EN/Research/ModellingSimulation/QIP/QTRL/_node.html)

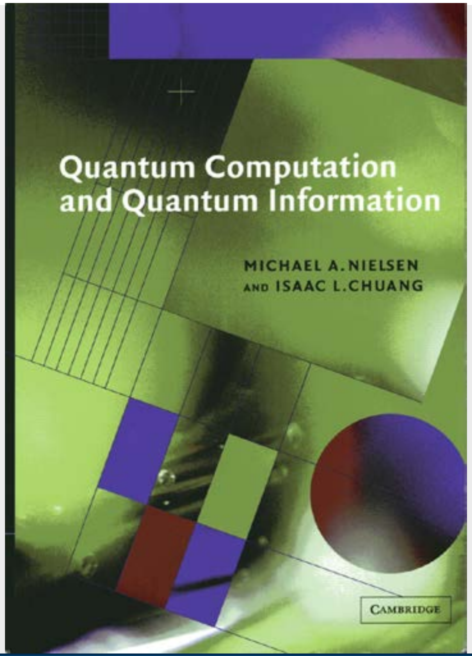
HOW TO EVALUATE QUANTUM COMPUTING

as a new compute technology?

We need profound test models and benchmarks to compare quantum computing / annealing devices with trustworthy simulations on digital supercomputers !

- Quantum Simulators
- Quantum Gate Based Systems
- Quantum Annealers

Test models / Simulation



QUANTUM COMPUTER IN THE MATHEMATICAL WORLD

Gate-based quantum computer: pen-and-paper (PaP) version

QUANTUM COMPUTER & QUANTUM ALGORITHM

- **Quantum computer**
  - System with 1 qubit ≡ system with 1 spin-1/2 particle

$$|\psi\rangle = a_0|0\rangle + a_1|1\rangle \quad ; \quad |a_0|^2 + |a_1|^2 = 1 \quad (a_0, a_1 \in \mathbb{C})$$

  - System with N qubits ≡ system with N spin-1/2 particles

$$|\psi\rangle = a(0\cdots 00)|0\rangle_{N-1}\cdots|0\rangle_1|0\rangle_0 + \cdots + a(1\cdots 11)|1\rangle_{N-1}\cdots|1\rangle_1|1\rangle_0$$

→ $|\psi\rangle$ can be represented as a vector of length 2^N, containing all complex amplitudes a

- **Quantum algorithm** = sequence of elementary operations (gates: X, Hadamard, CNOT, …) that change the state $|\psi\rangle$ of the quantum processor

WHERE DOES THE POWER OF THE PEN-AND-PAPER QC (PaP-QC) COME FROM?

- An operation of a PaP-QC amounts to multiplying the wave function with a unitary matrix
  - It is believed, without any empirical evidence, that Nature knows how to do such an operation in 1 step ⇔ many-world interpretation?

- It follows that the PaP-QC is a superb parallel computer that multiplies a $2^N \times 2^N$ matrix and a 2^N vector in 1 step
- In theory: exponential speed-up (order of 1 instead of 2^{2N} operations) for algorithms that can exploit this parallelism (hard to find!), e.g. Shor’s number factoring algorithm
- In practice: measurement of the outcome might destroy the parallelism

MEASUREMENT

- PaP-QC outputs $|\psi'\rangle = U|\psi\rangle$

  → all 2^N complex amplitudes $a_j; j = 0, \cdots, 2^{N-1}$ are known

  → all probabilities $|a_j|^2; j = 0, \cdots, 2^{N-1}$ can be calculated
- Measurement with a real gate-based QC device
  - In each measurement, every qubit is read-out returning a value 0 OR 1 for each qubit

    → Each measurement returns one of the 2^N basis states

    → Many measurements are required to determine $|a_j|^2; j = 0, \cdots, 2^{N-1}$ How many?

    → If each $a_j \neq 0$, then $2^N \times samples$ measurements are required
    Shor algorithm: small fraction of $a_j \neq 0$

JÜLICH QUANTUM COMPUTER SIMULATOR (JUQCS)

JUQUEEN, Jülich, Germany

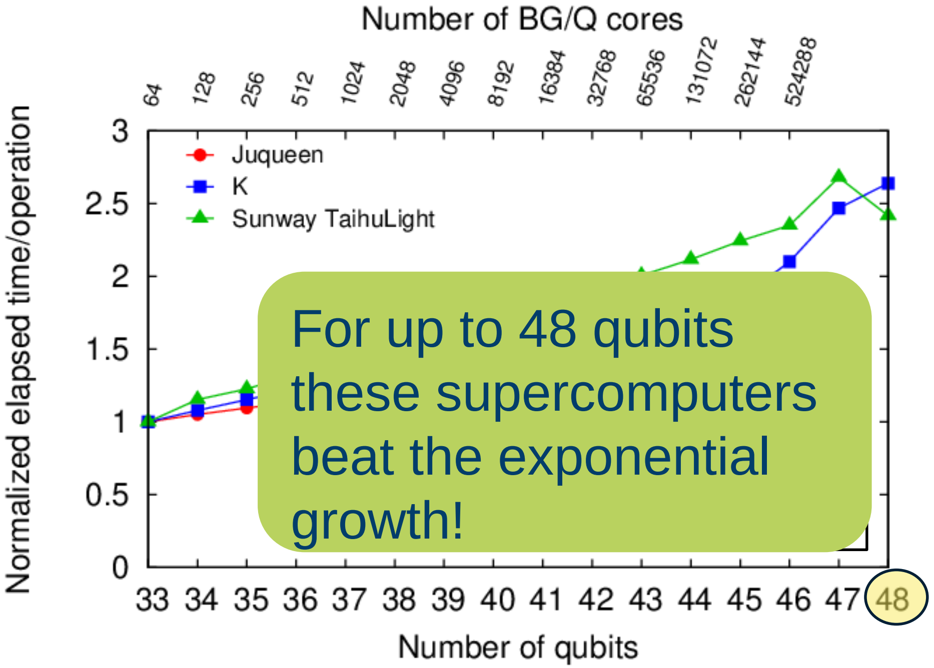
K, Kobe, Japan

Sunway TaihuLight, Wuxi, China

- N qubits → $|\psi\rangle$ is a superposition of 2^N basis states
- Represent a quantum state with 2 bytes → N qubits requires at least 2^{N+1} bytes of memory → new world record in 2018

N	Memory
27	256 MB
39	1 TB
48	0.5 PB
49*	1 PB

* Could be run on Trinity, Los Alamos



Test models / Simulation

QUANTUM COMPUTER IN THE MATHEMATICAL WORLD

Full dynamics of a quantum spin-1/2 system: gate-based quantum computer & quantum annealer

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QUANTUM COMPUTER / ANNEALER

- Quantum computer / annealer hardware can be modeled in terms of qubits that evolve in time (dynamics) according to the time-dependent Schrödinger equation (TDSE)

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

  - $|\psi(t)\rangle$: linear combination of all possible qubit states (2^N), describes the state of the whole quantum computer at time t
  - $H(t)$: time-dependent Hamiltonian modeling the quantum computer / annealer hardware and its control and eventually its interaction with the environment to model all kinds of errors

QUANTUM COMPUTER / ANNEALER

- Model for a universal quantum computer / annealer (spin-1/2 system):

$$H(t) = -\sum_{i=1}^{N} \sum_{\alpha=x,y,z} h_i^\alpha(t)\sigma_i^\alpha - \sum_{i,j=1}^{N} \sum_{\alpha=x,y,z} J_{ij}^\alpha(t)\,\sigma_i^\alpha\sigma_j^\alpha$$

where:

$$\sigma_i^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_i^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_i^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are the Pauli matrices and

J_{ij}: exchange interaction

h_i: magnetic field

QUANTUM ALGORITHMS

- Gate-based quantum computer: A quantum algorithm consists of a sequence of elementary operations (gates) that change the state $|\psi(t)\rangle$ of the quantum processor according to the TDSE.

- Quantum annealer: A quantum algorithm consists of the continuous time (natural) evolution of a quantum system to find the lowest-energy state of a system representing an optimization problem.

QUANTUM ANNEALING: HOW TO SOLVE AN OPTIMIZATION PROBLEM?

- Write the cost function $F = \sum_{i,j} Q_{ij} x_i x_j$ with $x_i \in \{0,1\}$ as Hamiltonian (energy function) of the Ising model such that its lowest-energy state represents the solution to the optimization problem (QUBO)

$$H_P = -\sum_{i=1}^{N} h_i s_i - \sum_{i,j} J_{i,j} s_i s_j$$

  with $s_i \in \{-1, +1\}$ and

  $J_{i,j}$: exchange interaction

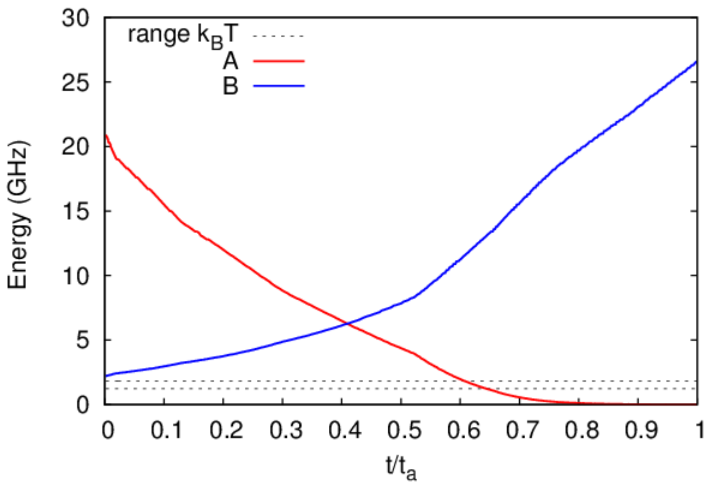
  h_i: external magnetic field

- Add a term H_I representing quantum fluctuations to induce quantum transitions between the states

QUANTUM ANNEALING: HOW TO SOLVE AN OPTIMIZATION PROBLEM?

- Quantum annealing = continuous time (natural) evolution of a quantum system described by the Hamiltonian

$$H(t) = A(t)H_I + B(t)H_P$$

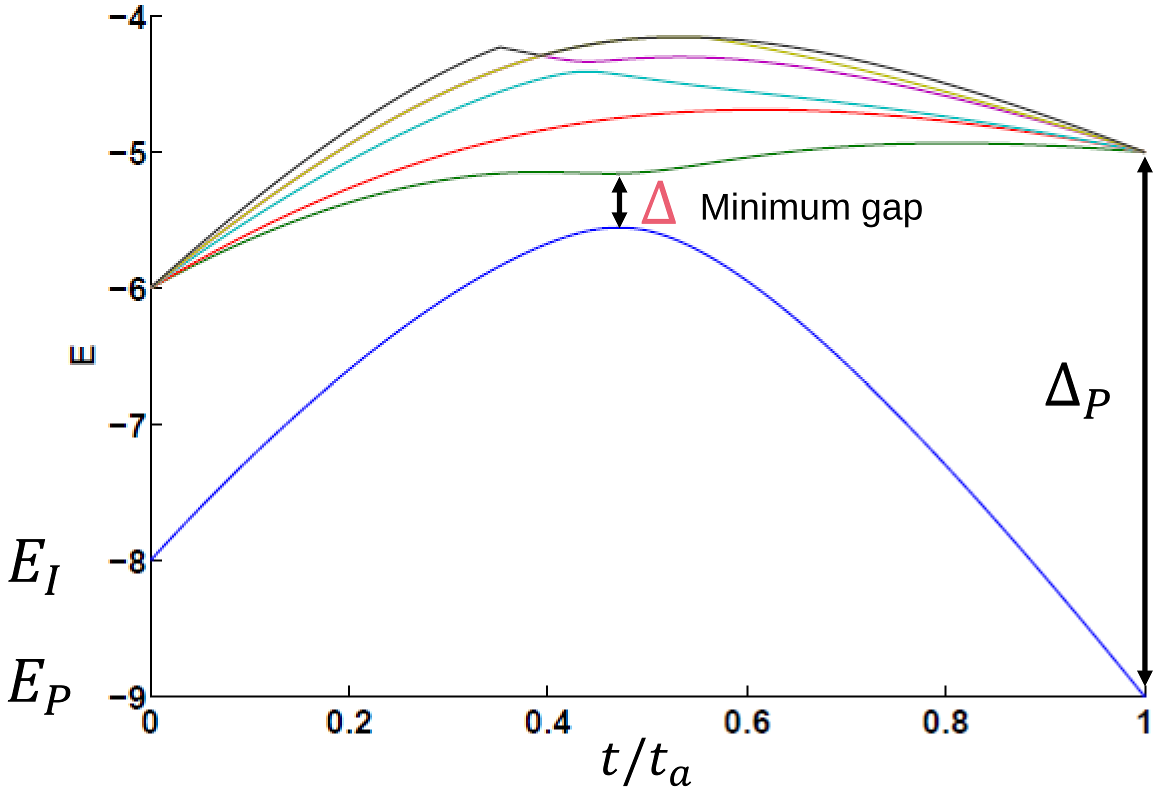


in the time period $0 \leq t \leq t_a$

- The total Hamiltonian changes from H_I at $t = 0$ to H_P at $t = t_a$
- At $t = 0$ the system is prepared in the lowest energy state of H_I
- If the time evolution is adiabatic, then at $t = t_a$ the system is in the lowest-energy state of H_P → the solution of the optimization problem has been found

QUANTUM ANNEALING

- Quantum theoretical description of the quantum annealing process: Landau-Zener theory



Energy spectrum of the lowest lying states

Landau-Zener formula: probability to remain in the lowest energy state during annealing

$$P = 1 - e^{-\alpha t_a \Delta^2}$$

$$t_a \to \infty : P = 1$$
$$t_a \to 0 : P = 0$$

Benchmarking

QUANTUM COMPUTERS IN THE WORLD THAT HUMANS EXPERIENCE

SIMULATION ON IBM QUANTUM EXPERIENCE (IBM QX)

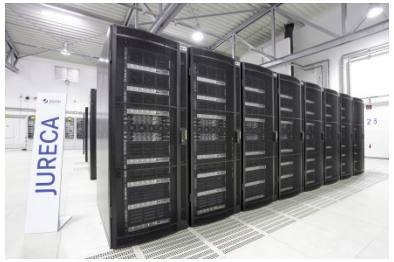
IBM QX, Yorktown Heights, USA

- The IBM QX processor with 5 and 16 qubits can be tested freely from “outside” the lab
  - Allows for an independent assessment of a quantum processor as a computing device
- We tested the performance of the IBM QX processors
  - Simple algorithms: identity operations, 2+2 qubit adder, measurement of singlet state, error correction

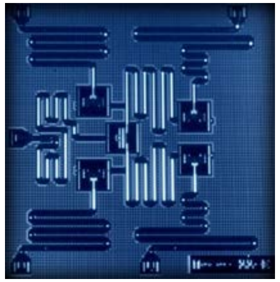
General conclusion: The current IBM QX device does not meet the elementary requirements for a computing device.

K. Michielsen, M. Nocon, D. Willsch, F. Jin, Th. Lippert, H. De Raedt, *Benchmarking gate-based quantum computers*, Comp. Phys. Comm. 220, 44 (2017)

SIMULATION ON/OF SYSTEMS WITH TWO TRANSMON QUBITS

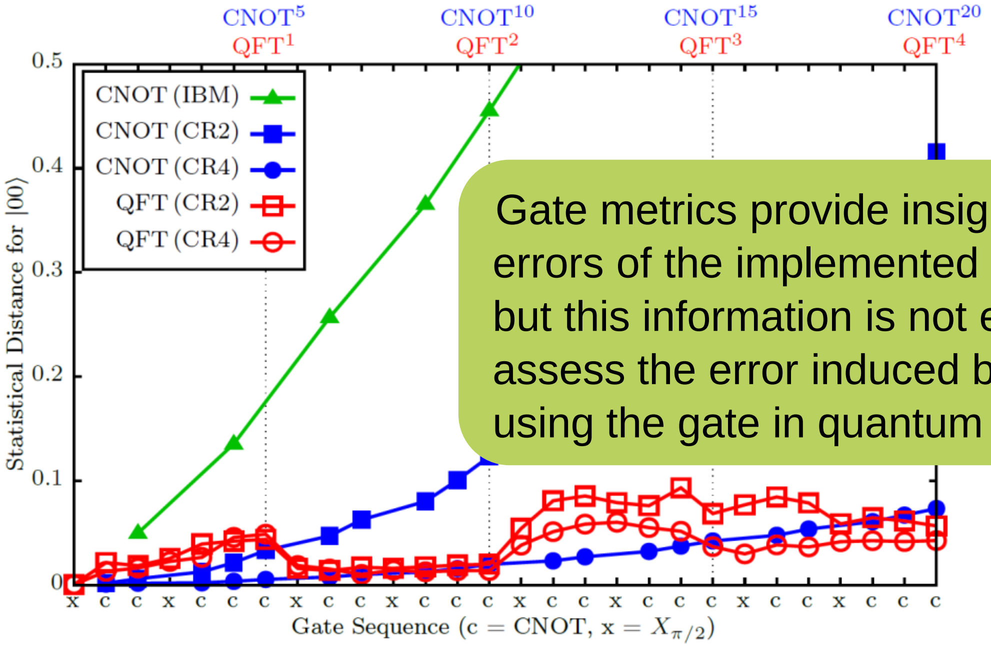


JURECA, Jülich, Germany



IBM QX, Yorktown Heights, USA

- Simulation of the real-time dynamics of physical models of systems with two transmon qubits
- Comparison with IBM QX1 device



Gate metrics provide insights into errors of the implemented gate pulses, but this information is not enough to assess the error induced by repeatedly using the gate in quantum algorithms.

D. Willsch, M. Nocon, F. Jin, H. De Raedt, K. Michielsen, *Gate error analysis in simulations of quantum computers with transmon qubits*, Phys. Rev. A 96, 062302 (2017)

SIMULATION ON/OF D-WAVE QUANTUM ANNEALERS

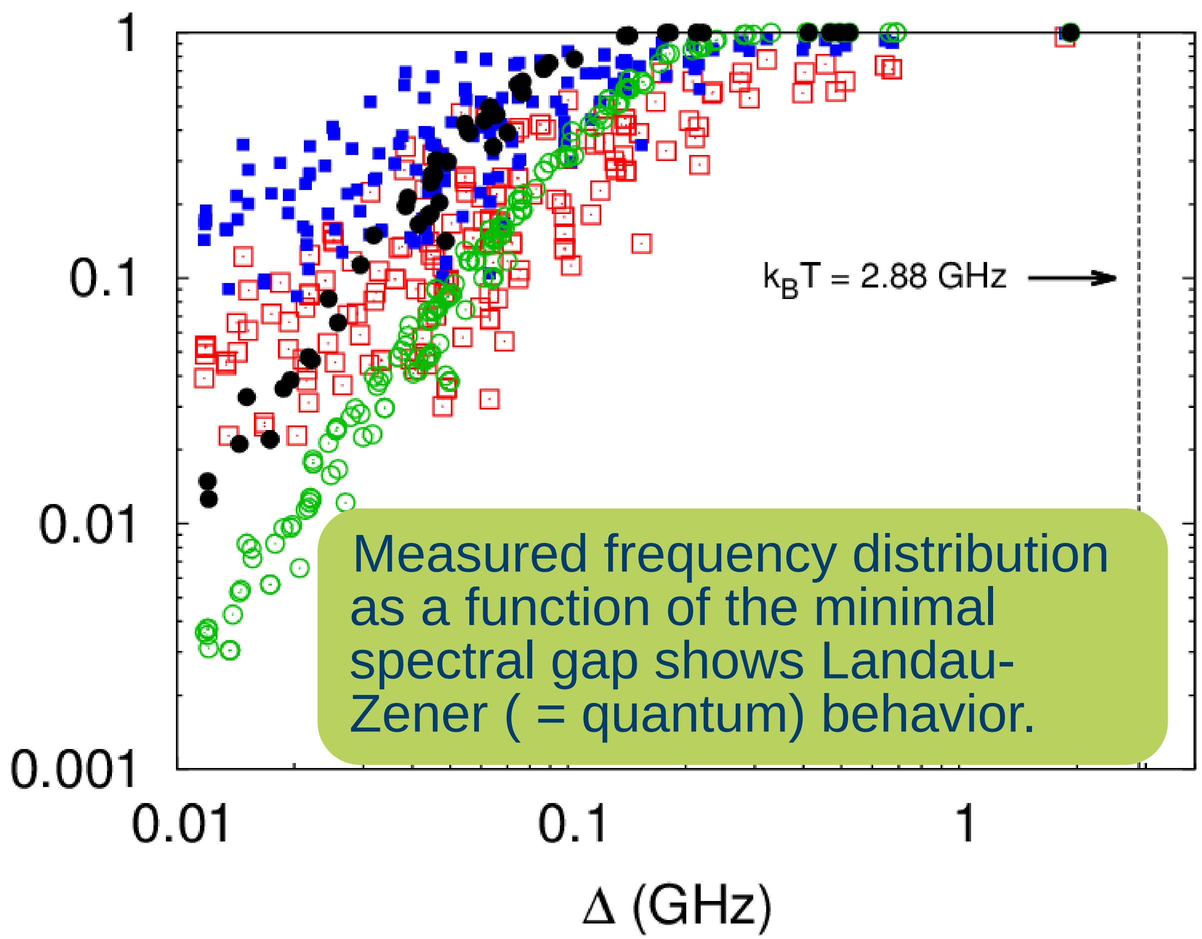
D-Wave, Burnaby, Canada

- Comparison test for the analysis and exploration of D-Wave quantum annealers
  - Solve small but hard Ising problems, characterized by a known unique ground state and a highly degenerate first excited state, on a D-Wave system and on a simulated ideal quantum annealer modeled as a quantum spin-1/2 system
    - Use problems that can be directly mapped on the Chimera architecture
    - Use D-Wave system parameters for the simulation

K. Michielsen, F. Jin, and H. De Raedt, *Solving 2-satisfiability problems on a quantum annealer* (in preparation)

SIMULATION ON/OF D-WAVE QUANTUM ANNEALERS

D-Wave, Burnaby, Canada



Measured frequency distribution as a function of the minimal spectral gap shows Landau-Zener (= quantum) behavior.

K. Michielsen, F. Jin, and H. De Raedt, *Solving 2-satisfiability problems on a quantum annealer* (in preparation)

QUANTUM COMPUTER USER FACILITY JUNIQ AND USER GROUP EQUIPE

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PRACTICAL USAGE OF QUANTUM COMPUTERS, A CASTLE IN THE AIR ?

BUILDING CASTLES IN THE AIR IS USELESS UNLESS WE HAVE A LADDER TO REACH THEM

Matshona Dhliwayo

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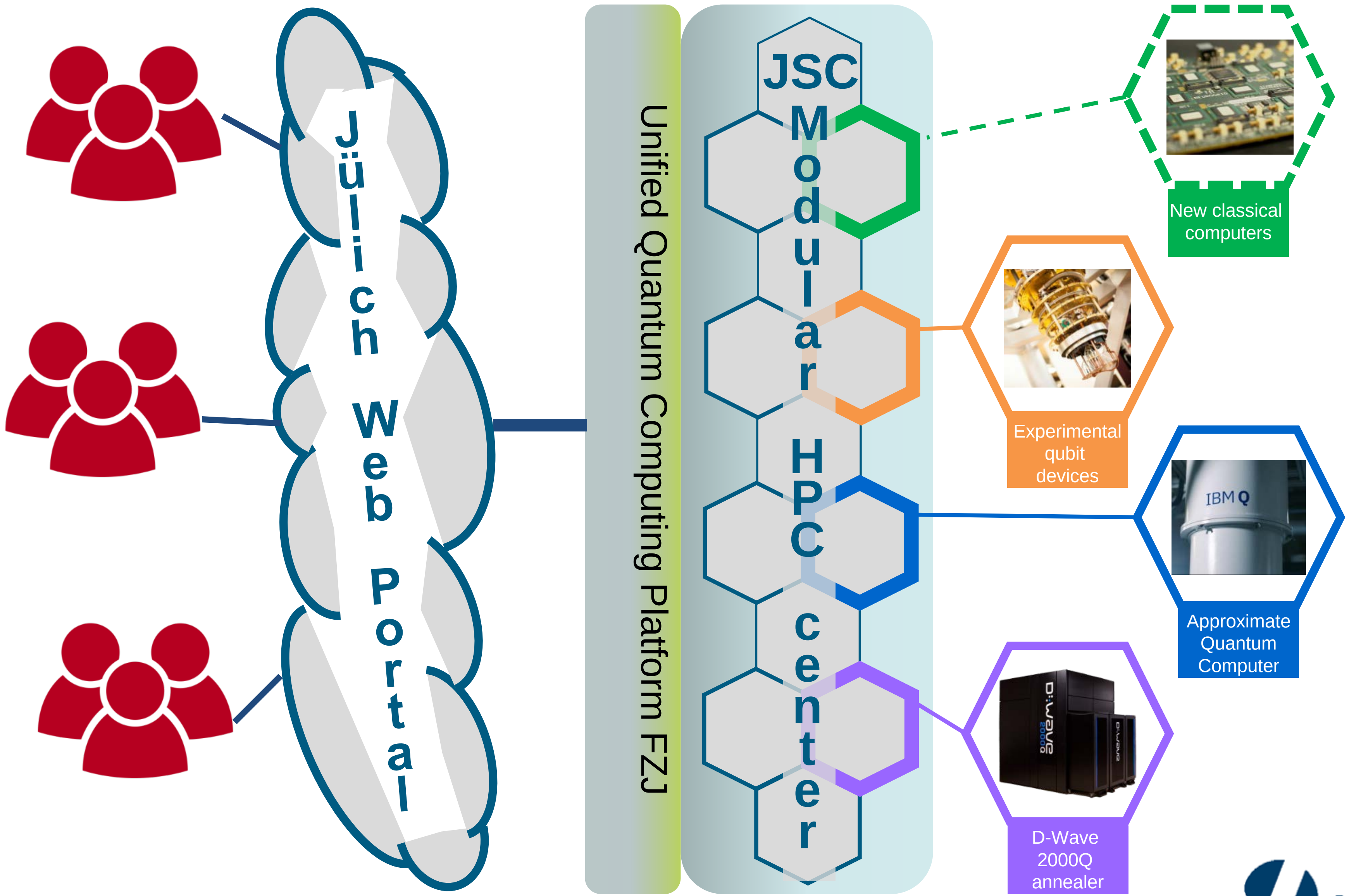
QC USER FACILITY JUNIQ AND USER GROUP EQUIPE

- Establish a QC User Facility JUNIQ and provide
  - affordable and barrier-free access to available computing devices for users in science and industry in Europe - Create a maturity ramp of systems available
    - QTRL 8 Host and operate annealers exploiting quantum phenomena
    - QTRL 4-5 Provide access to multi-qubit devices for quantum computing without error correction (e.g. IBM, Google, Rigetti Computing)
    - QTRL 2-3 Provide access to experimental devices
  - access to quantum computer simulators (JUQCS, ATOS QLM)
  - high level user support in all aspects of high performance and quantum computer usage
- Establish a user group EQUIPE to enable quantum information processing in Europe

QUANTUM COMPUTER USER FACILITY JUNIQ



CONCLUSIONS

CONCLUSIONS

- Simulating the behavior of (physical models) of quantum computing devices (D-Wave, IBM, …) on supercomputers sheds light on the physical processes involved

- Applications for currently available gate-based quantum computers (< 50 qubits) CAN be tested on supercomputers
- Applications for currently available quantum annealers (> 2000 qubits) CANNOT be tested on supercomputers
  - Simulation time required to simulate small quantum annealing problems (≈ 20 qubits) is much larger than the physical annealing time (≈ 20 μs)
- Establishment of user facility JUNIQ and user group EQUIPE

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