QUANTUM COMPUTING APPLICATIONS AT JSC

JÜLICH UNIFIED INFRASTRUCTURE FOR QUANTUM COMPUTING (JUNIQ)

22 MARCH 2023 I DR. DENNIS WILLSCH

Member of the Helmholtz Association

WE COMPUTE WITH QUANTUM COMPUTERS

supported by Bundesministerium für Bildung und Forschung

Ministerium für Kultur und Wissenschaft des Landes Nordrhein-Westfalen

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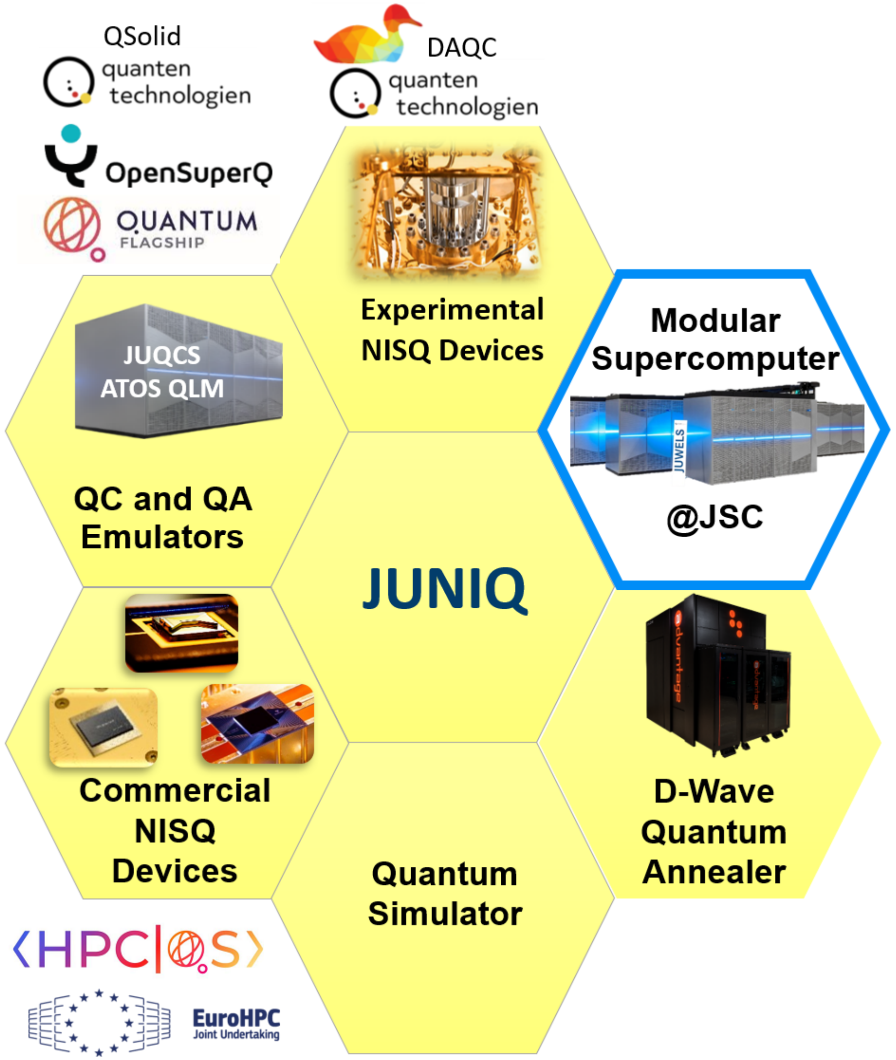
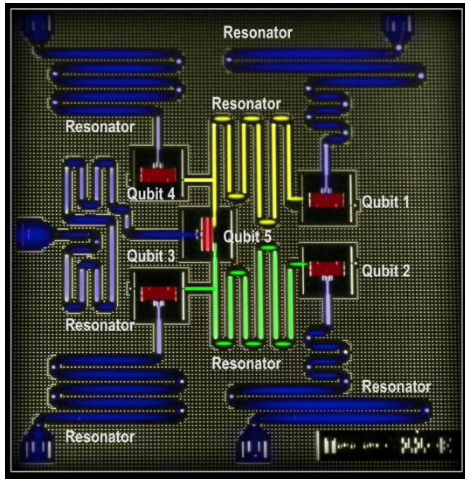
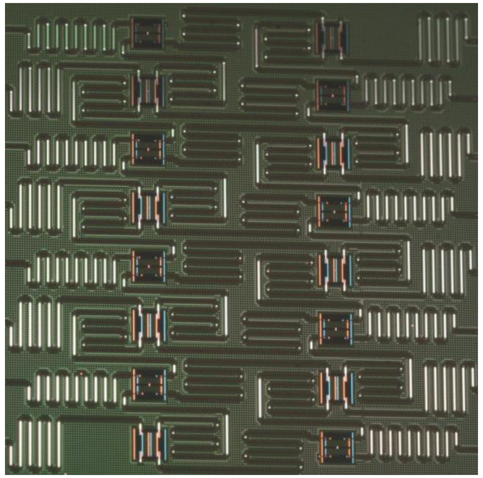


QUANTUM COMPUTERS

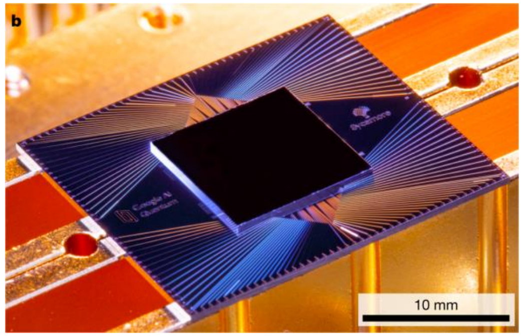
Two main paradigms: Gate-based QC and Quantum Annealing

IBM: 1, 5, 7, 16, 27, 65, 127, 433 Qubits

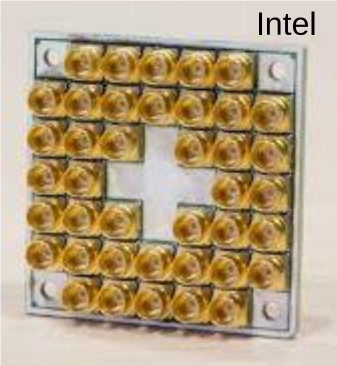




Google: 53, 72 Qubits

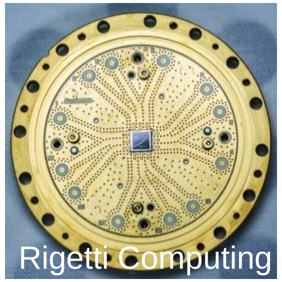


Intel: 17, 49 Qubits

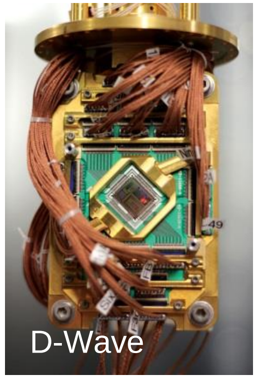


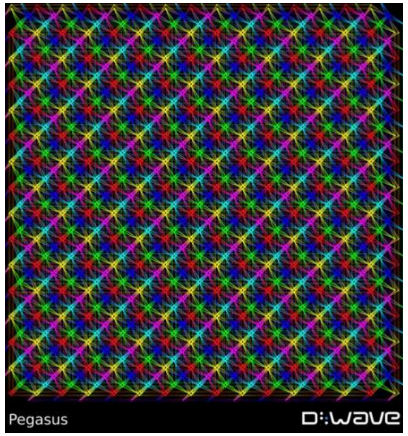
Rigetti Computing:

8, 16, 19 Qubits



D-Wave: 2048, 5760 Qubits



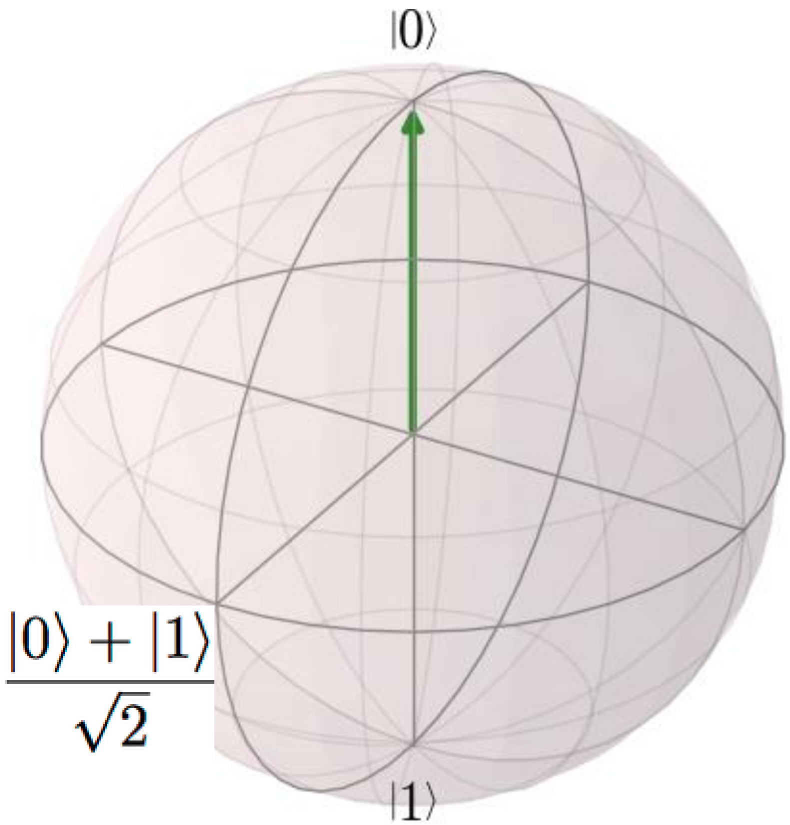


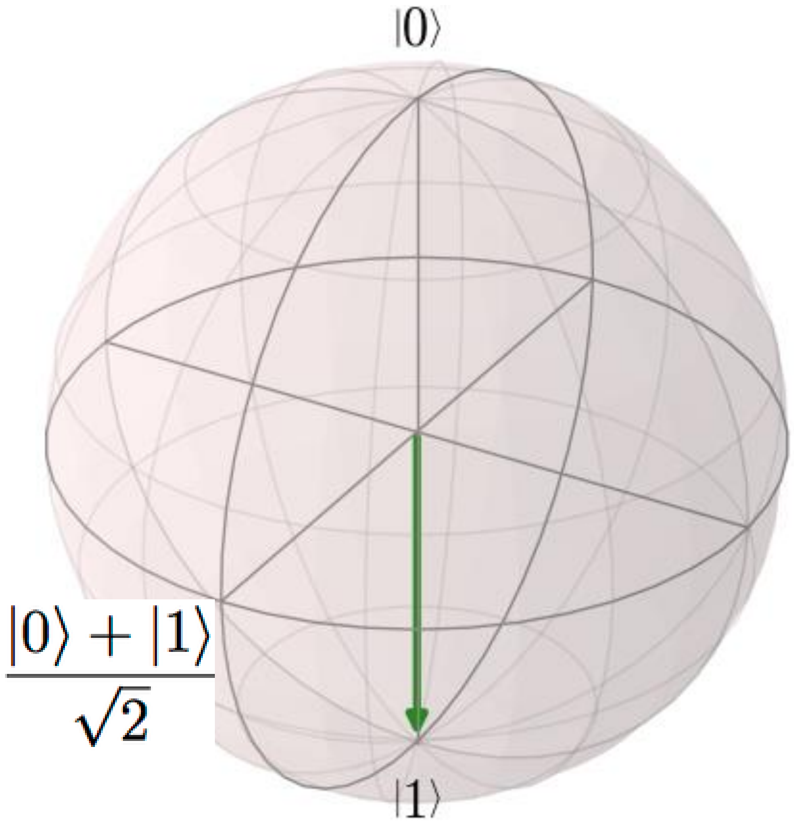
WHAT IS A QUBIT?

Digital Computer: Bit

Quantum Computer: Quantum Bit = Qubit

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



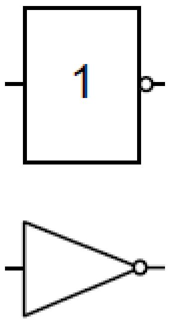


GATE-BASED QUANTUM COMPUTING

Digital Gates:

1 bit:

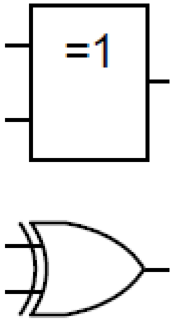
NOT



a	y
0	1
1	0

2 bits:

XOR



a	b	y
0	0	0
0	1	1
1	0	1
1	1	0

... and many more

Quantum Gates

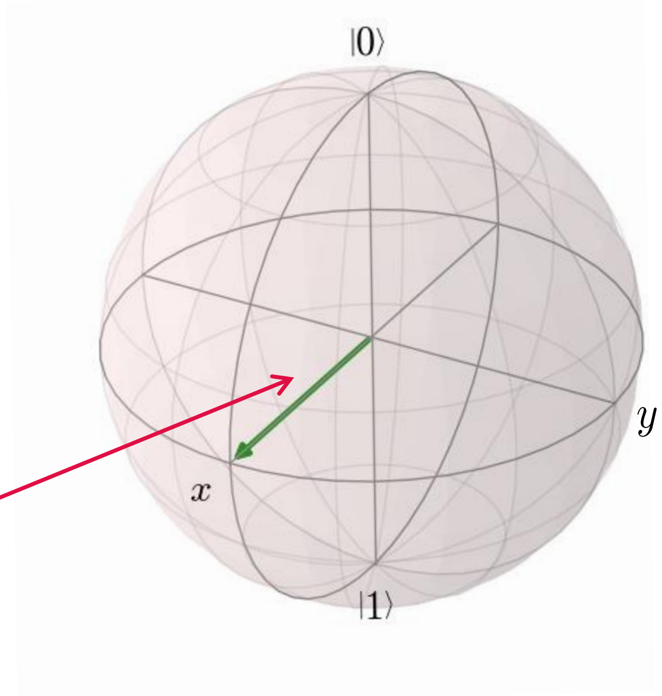
1 qubit: $\alpha|0\rangle + \beta|1\rangle$

X-Gate (NOT): $|0\rangle$ — X — $|1\rangle$

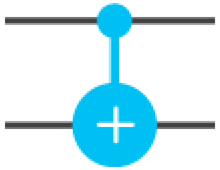
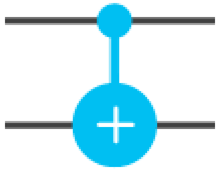
Y-Gate (i-NOT): $|0\rangle$ — Y — $i|1\rangle$

Hadamard (H): $|0\rangle$ — H — $\frac{|0\rangle+|1\rangle}{\sqrt{2}}$

... and many more

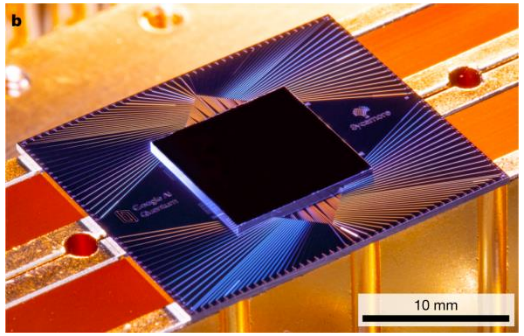


2 qubits: $\alpha|00\rangle + \beta|01\rangle + \gamma|10\rangle + \delta|11\rangle$

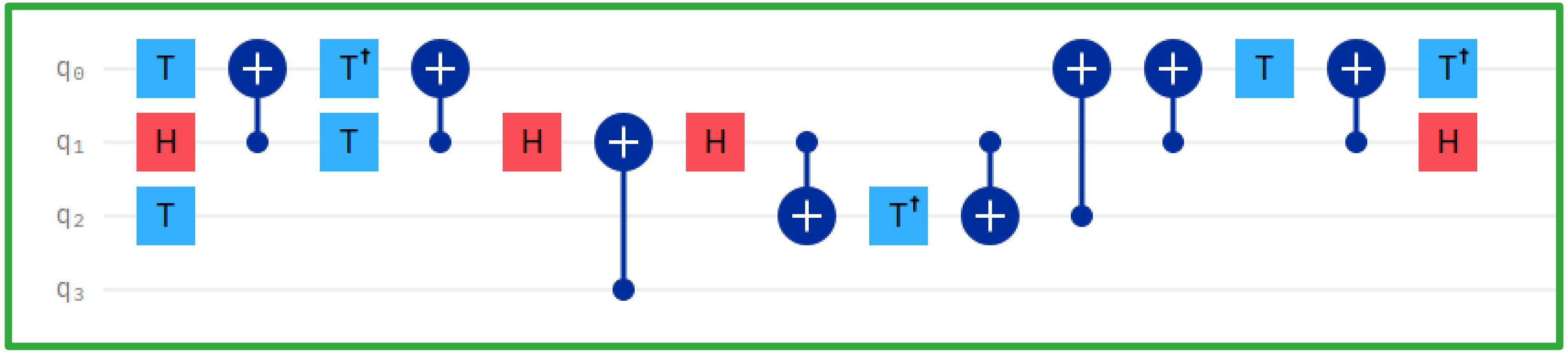
CNOT: $|00\rangle$  $|00\rangle$ $|10\rangle$  $|11\rangle$

GATE-BASED QUANTUM COMPUTING

The Idea



- What does a gate-based quantum computer do?
  - It runs a quantum circuit



- What does this mean, actually?
  - It performs **matrix-vector multiplications** that are

sparse **complex** **unitary**

  - with **huge** vectors and **huge²** matrices

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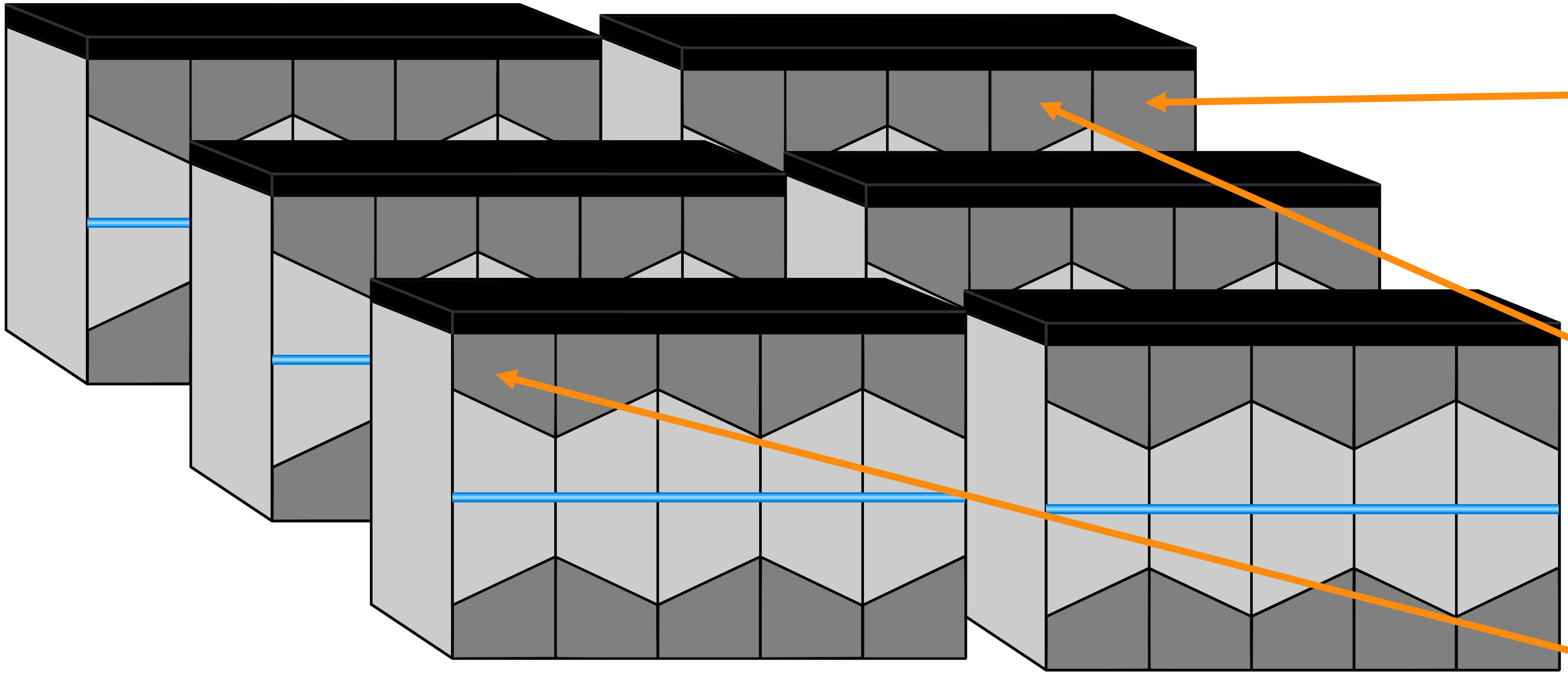
De Raedt et al., CPC **176**, 121 (2007)
De Raedt et al., CPC **237**, 47 (2019)
Willsch et al., CPC **278**, 108411 (2022)

GATE-BASED QUANTUM COMPUTING

Simulating with JUQCS (Jülich Universal Quantum Computer Simulator)



GPU #0 (Node #0)

$$\begin{pmatrix} \psi_{00000000000\,0\cdots0} \\ \vdots \\ \psi_{00000000000\,1\cdots1} \end{pmatrix}$$

GPU #4 (Node #1)

$$\begin{pmatrix} \psi_{00000000001\,0\cdots0} \\ \vdots \\ \psi_{00000000001\,1\cdots1} \end{pmatrix}$$

GPU #2047

$$\begin{pmatrix} \psi_{11111111111\,0\cdots0} \\ \vdots \\ \psi_{11111111111\,1\cdots1} \end{pmatrix}$$

- **Video:** Simulation of Quantum Computers on GPUs
  https://www.youtube.com/watch?v=JUSEYCkh2ac
- **JUNIQ:** Possible to simulate around 40 qubits (45 with JUQCS)
  https://juniq.fz-juelich.de

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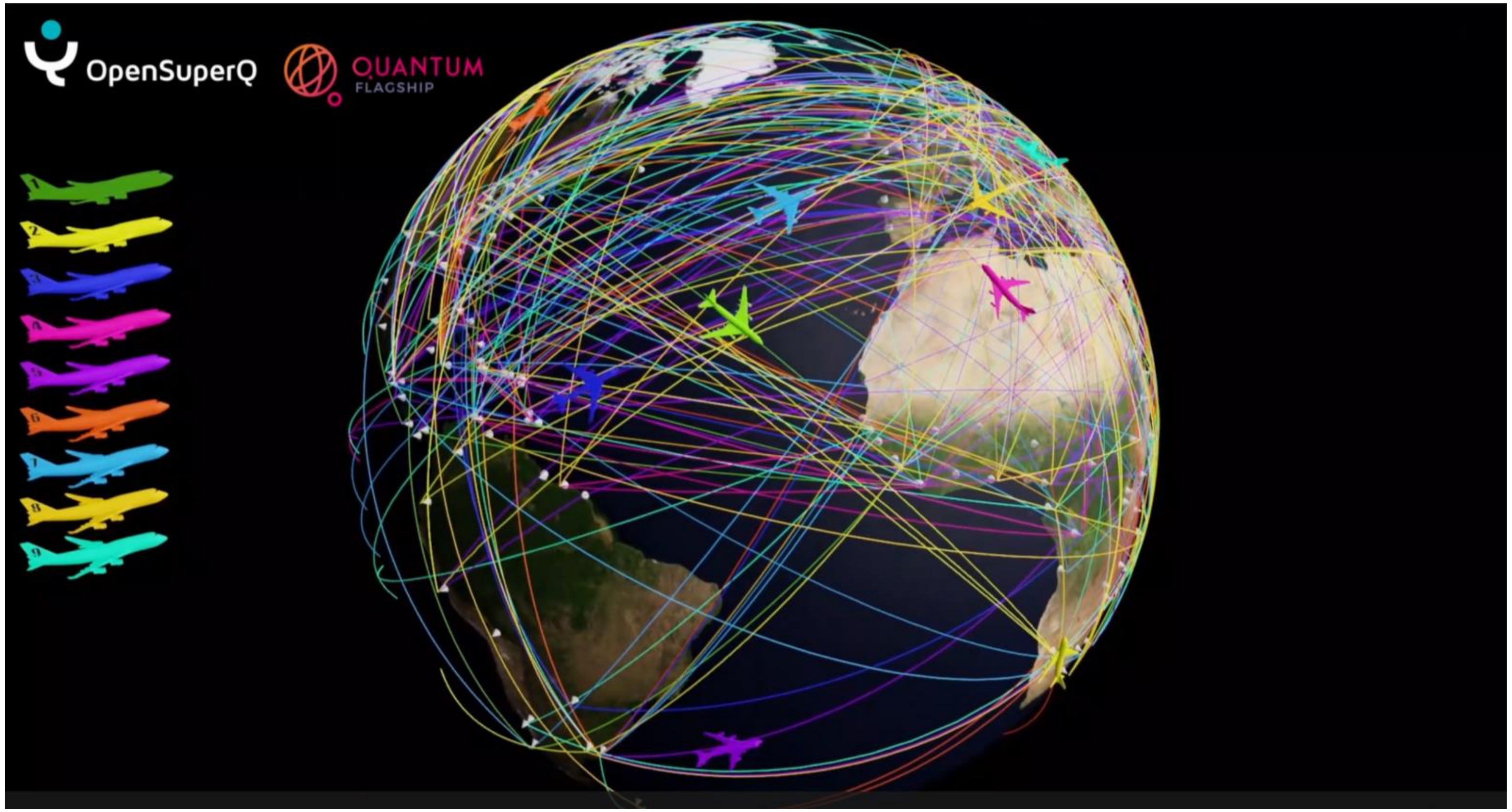
Willsch et al. (2022)
CPC **278**, 108411
arXiv:2104.03293

GATE-BASED QUANTUM COMPUTING

Application: Tail Assignment (Airline Scheduling)

Find optimal flight schedule such that each flight is covered exactly once



<u>In collaboration with:</u>
Marika Svensson
Jeppesen and
Chalmers University of Technology

BOEING
OpenSuperQ
QUANTUM FLAGSHIP

Willsch et al. (2022)
CPC **278**, 108411
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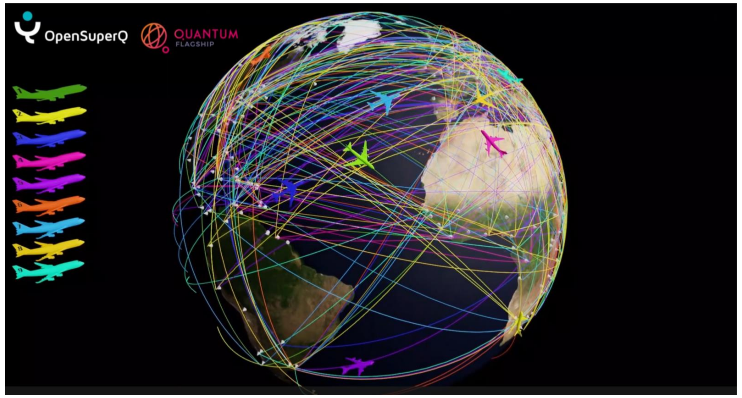
GATE-BASED QUANTUM COMPUTING

Application: Tail Assignment (Airline Scheduling)



Find optimal flight schedule
such that each flight is covered
exactly once

	Flight 0	Flight 1	Flight 2	Flight 3	Flight 4	Flight 5	⋯	Flight 469	Flight 470	Flight 471
Route 0	0	1	0	0	0	0		0	0	0
Route 1	0	0	0	0	1	0		0	0	0
⋮										
Route 10	0	0	0	0	0	1		0	0	1
Route 11	0	0	1	0	0	0		0	0	0
Route 12	0	0	0	1	0	0		1	0	0
Route 13	0	0	1	0	0	0		0	0	0
Route 14	0	0	0	1	0	0		0	0	0
Route 15	0	0	0	0	1	0		0	0	0
Route 16	0	1	0	0	0	0		0	1	0
⋮										
Route 37	0	0	0	0	0	1		0	0	0
Route 38	0	0	0	1	0	0		0	0	0
Route 39	0	0	0	1	0	0		0	0	0

→ Solved using QAOA with 40 qubits (on JUQCS)

QUANTUM ANNEALERS

What do they do?

Quadratic Unconstrained Binary Optimization

"bias" (real number)

$$\textbf{QUBO:}\quad \min_{x_i=0,1}\left(\sum_i a_i x_i + \sum_{i<j} b_{ij} x_i x_j\right)$$

problem variables (binary)

"coupler" (real number)

Why might this be interesting?
→ discrete optimization is **hard** (NP-hard)
→ produces **many solutions** simultaneously
→ very **low energy** consumption

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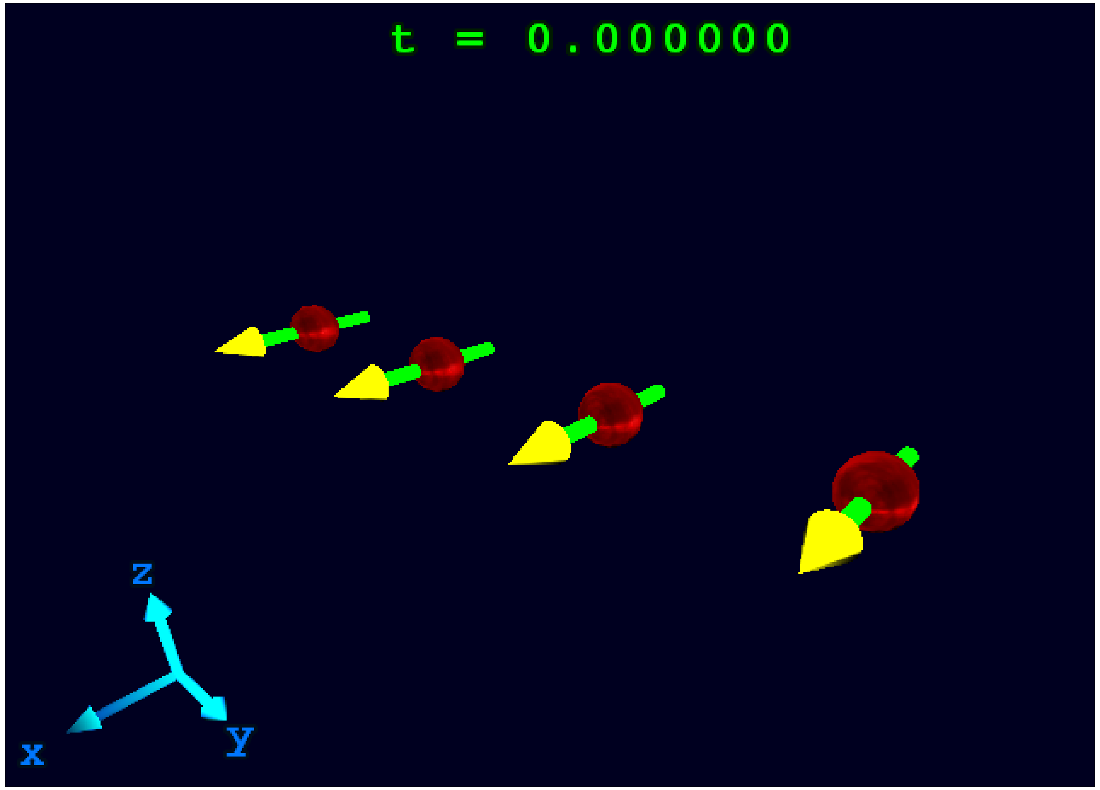
QUANTUM ANNEALERS

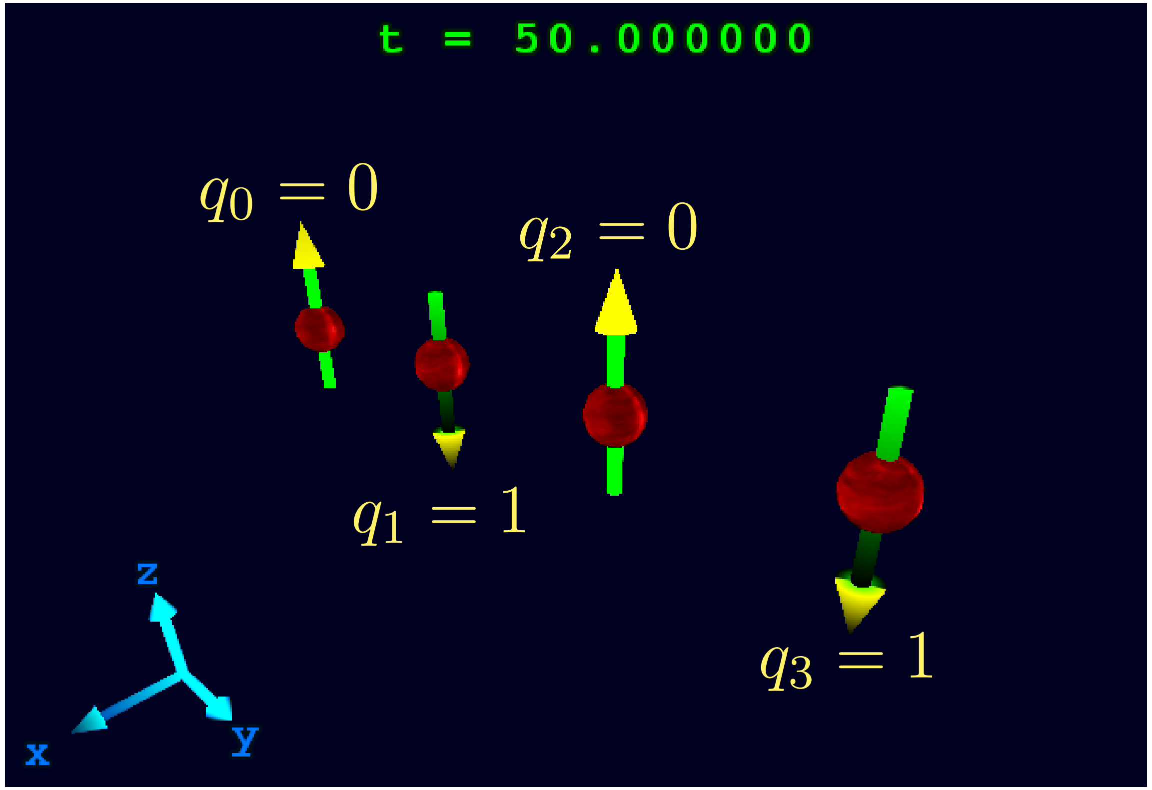
How do they work?

$$\text{QUBO}: \quad \min_{q_0 q_1 q_2 q_3} \left(\sum_i a_i q_i + \sum_{i<j} b_{ij} q_i q_j \right) \quad = \quad ????$$

Before the annealing process



After the annealing process



Quantum Annealing

QUANTUM ANNEALERS: APPLICATIONS

Video:
https://youtu.be/ieEXs9gbioY

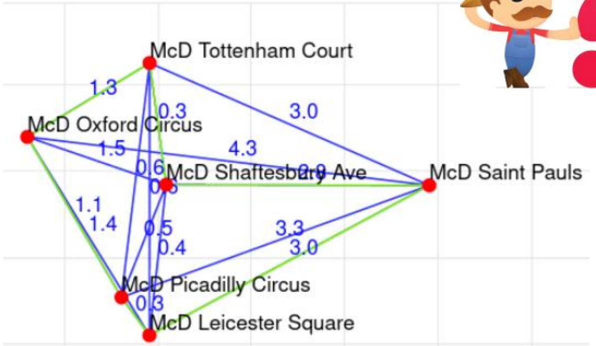
1. Airline Scheduling
2. Traveling Salesman
3. Garden Optimization
4. 2-Satisfiability
5. QSVM
6. QBM

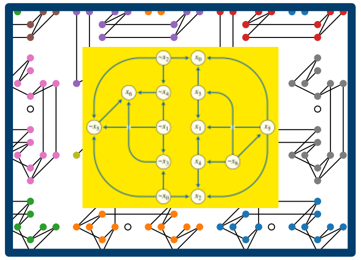
optimization problem with constraints [increasing complexity]

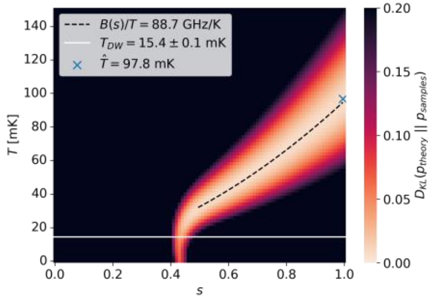
constraints only

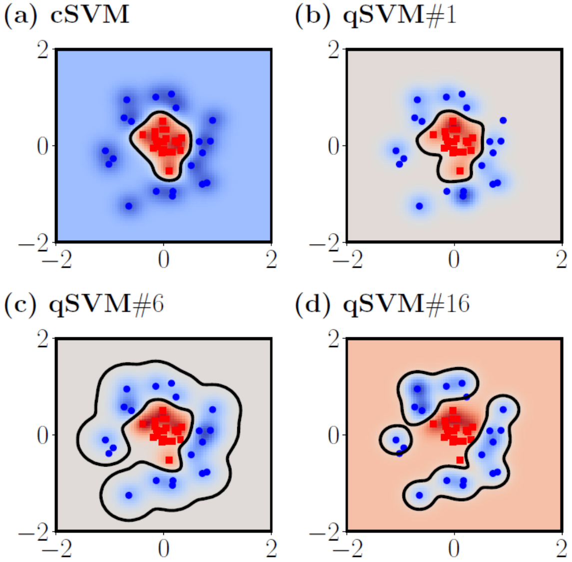
optimization only [basically]

sampling problem









JUNIQ Rolling Call:

or search for
"FZJ JUNIQ ACCESS"

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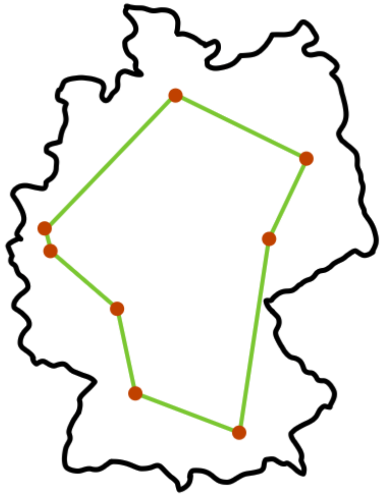
QUANTUM ANNEALERS: APPLICATIONS

Traveling Salesman Problem



$$\min_{x_i=0,1}\left(\sum_i a_i x_i + \sum_{i<j} b_{ij} x_i x_j\right)$$

Cost to travel from city i to city j

$$\min_{x_{it}=0,1}\left\{\lambda \sum_{i=0}^{n-1}\sum_{\substack{j=0\\ j\neq i}}^{n-1}\sum_{t=0}^{n-1} c_{ij}x_{it}x_{j(t+1)} + \sum_{i=0}^{n-1}\left(\sum_{t=0}^{n-1}x_{it}-1\right)^2 + \sum_{t=0}^{n-1}\left(\sum_{i=0}^{n-1}x_{it}-1\right)^2\right\}$$

time steps

cities

	0	1	2	3
A	1	0	0	0
B	0	0	0	1
C	0	1	0	0
D	0	0	1	0

- Assign cities & times to qubits:
  - Qubit $x_{it}=1$ means the traveler is at city i at time t
  - Count the cost c_{ij} if the traveler goes from i to j at some time step
  - Traveler must pass city i only once
  - Traveler can only be at one city at each time step
- Not the DFJ formulation: linear but exp. many inequality constraints
- Could simplify by fixing starting point
  → Number of qubits $(n-1)^2$

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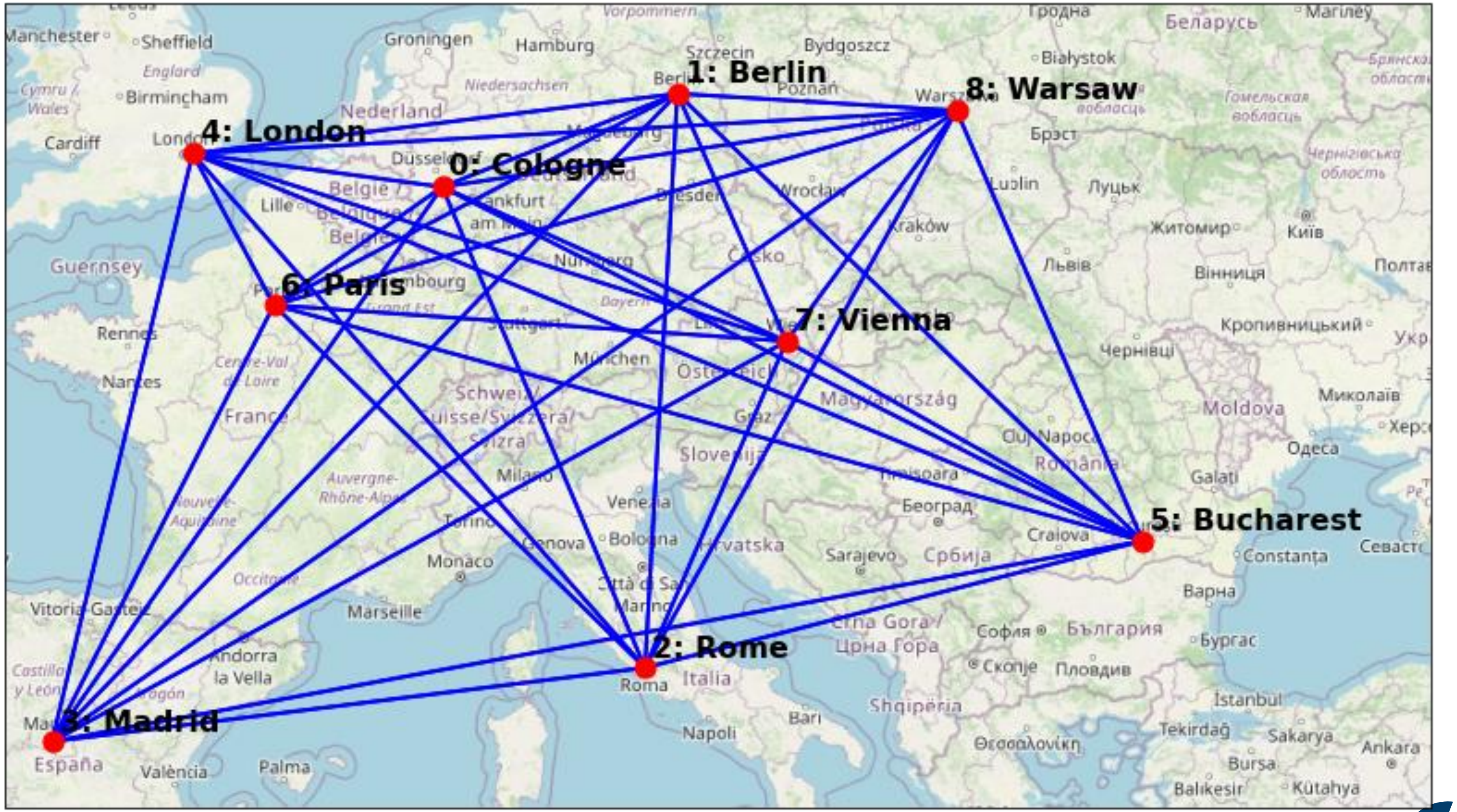
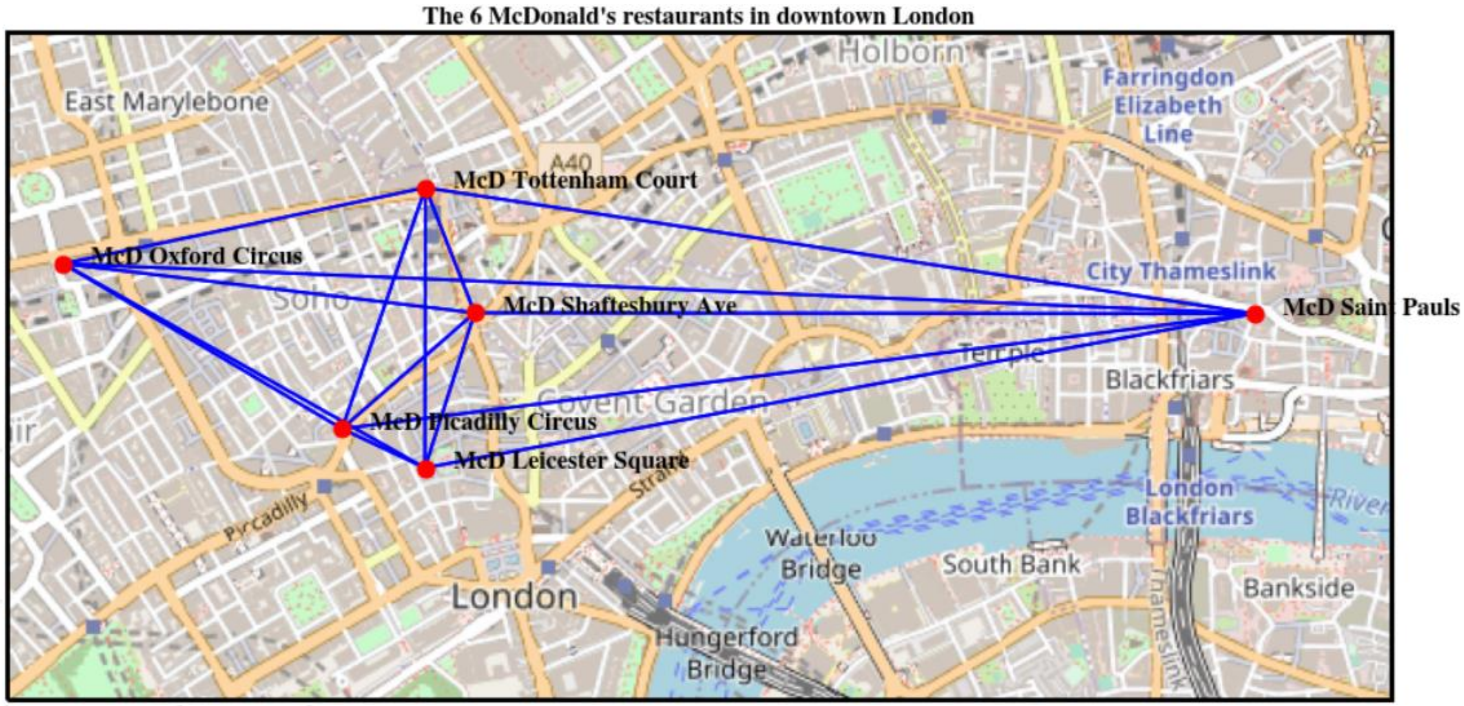
QUANTUM ANNEALERS

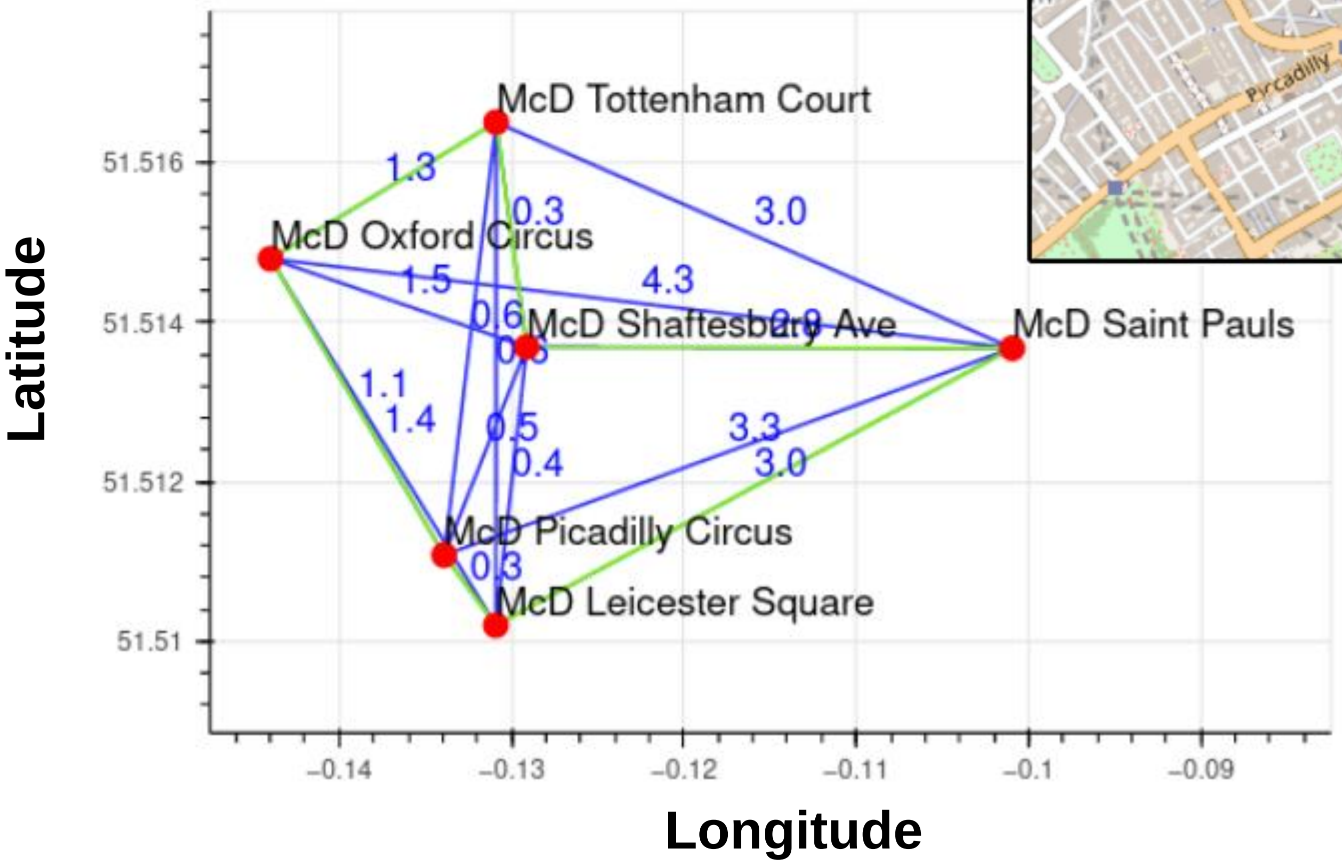
Traveling Salesman Problem



QUANTUM ANNEALERS

Traveling Salesman Problem





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Willsch et al., CPC 248, 107006 (2020)
Cavallaro et al., IGARSS 2020, 1973 (2020)
Delilbasic et al., IGARSS 2021, 2608 (2021)

QUANTUM ANNEALERS: APPLICATIONS

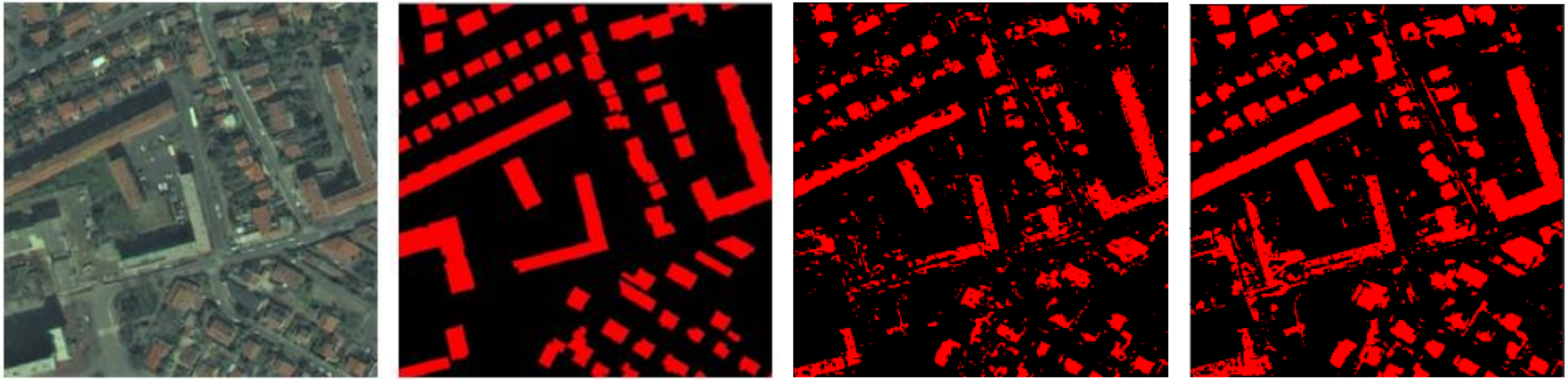
Quantum Support Vector Machines: Application to Remote Sensing

Willsch et al., CPC 248, 107006 (2020)
Cavallaro et al., IGARSS 2020, 1973 (2020)
Delilbasic et al., IGARSS 2021, 2608 (2021)

QUANTUM ANNEALERS: APPLICATIONS

Quantum Support Vector Machines: Application to Remote Sensing

False color | Ground truth | Classical SVM | Quantum SVM



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