Naïve QUBO Formulations

Jonas Nüßlein, Sebastian Zielinski,
Sebastian Feld, Claudia Linnhoff-Popien

IEEE Quantum Week (IEEE QCE'23)
September 18, 2023

Agenda

I. Quantum Annealing in a Nutshell

II. QGM vs. AQC

III. QUBO and TSP

IV. Satisfiability

V. PyQUBO

VI. Conclusion

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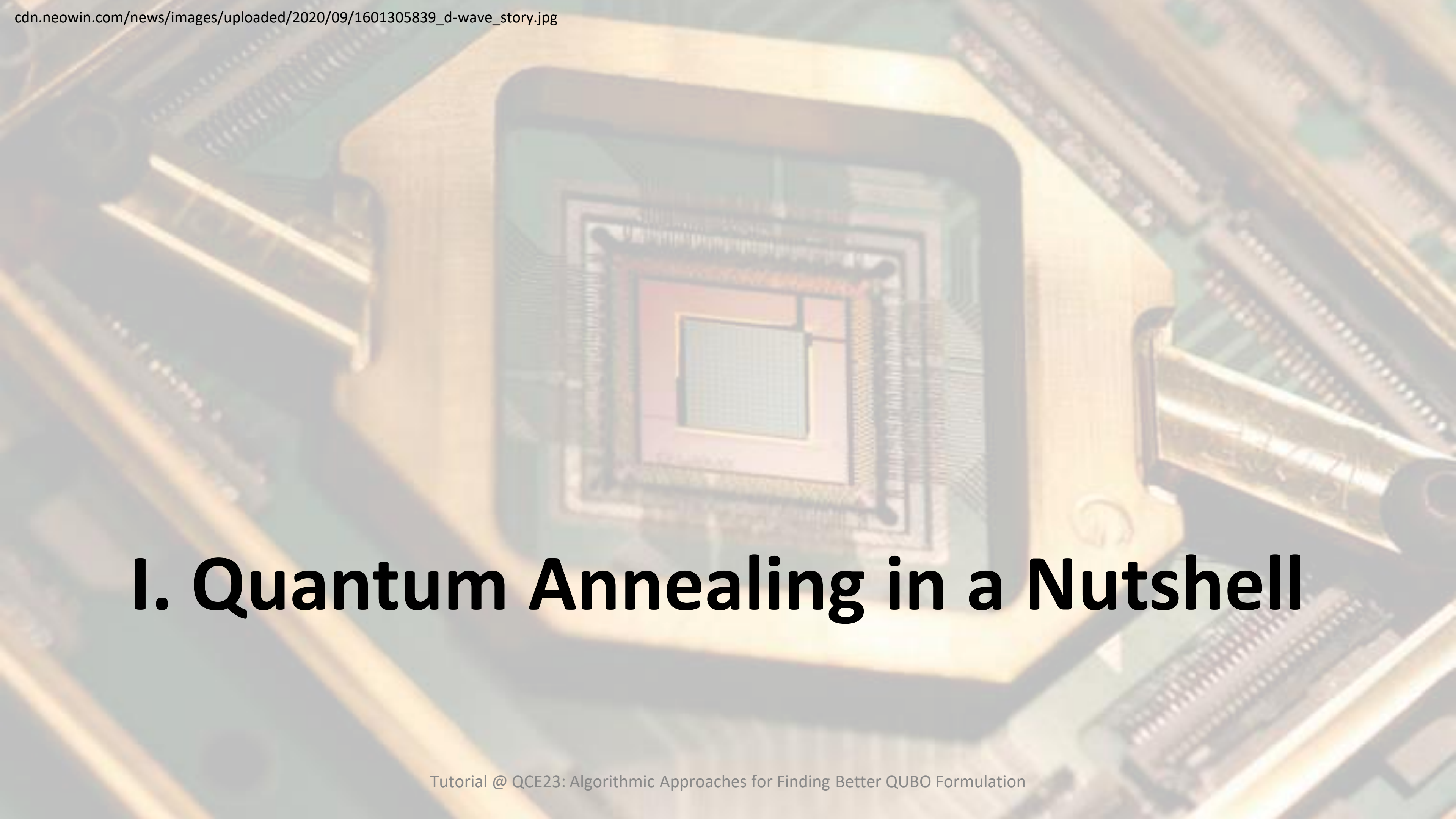


I. Quantum Annealing in a Nutshell

Quantum Computing

Quantum Gate Model

TU Delft

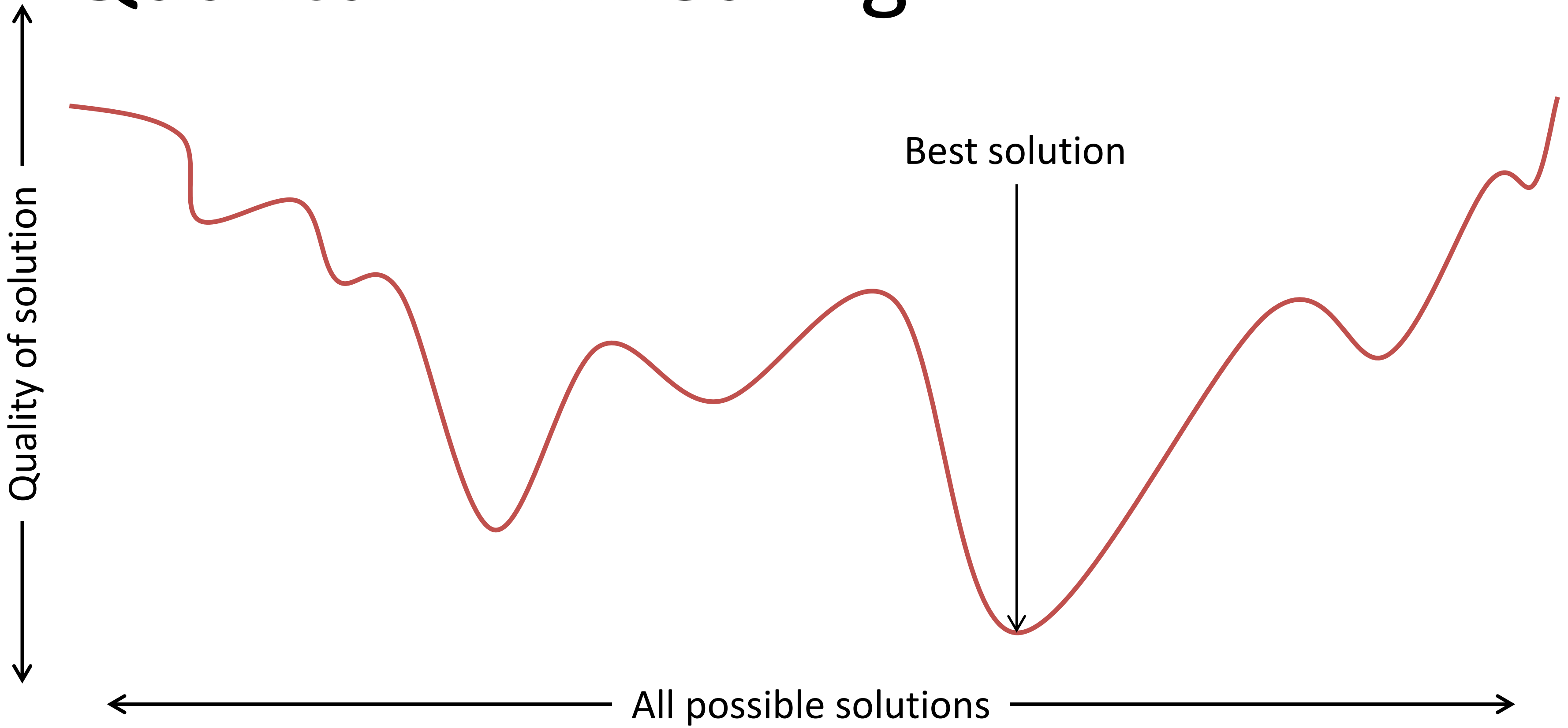
Google IBM Microsoft ...

Quantum Annealing

D:Wave

The Quantum Computing Company™

Quantum Annealing



Portfolio Optimization

					…	
?	?	?	?	?	…	?

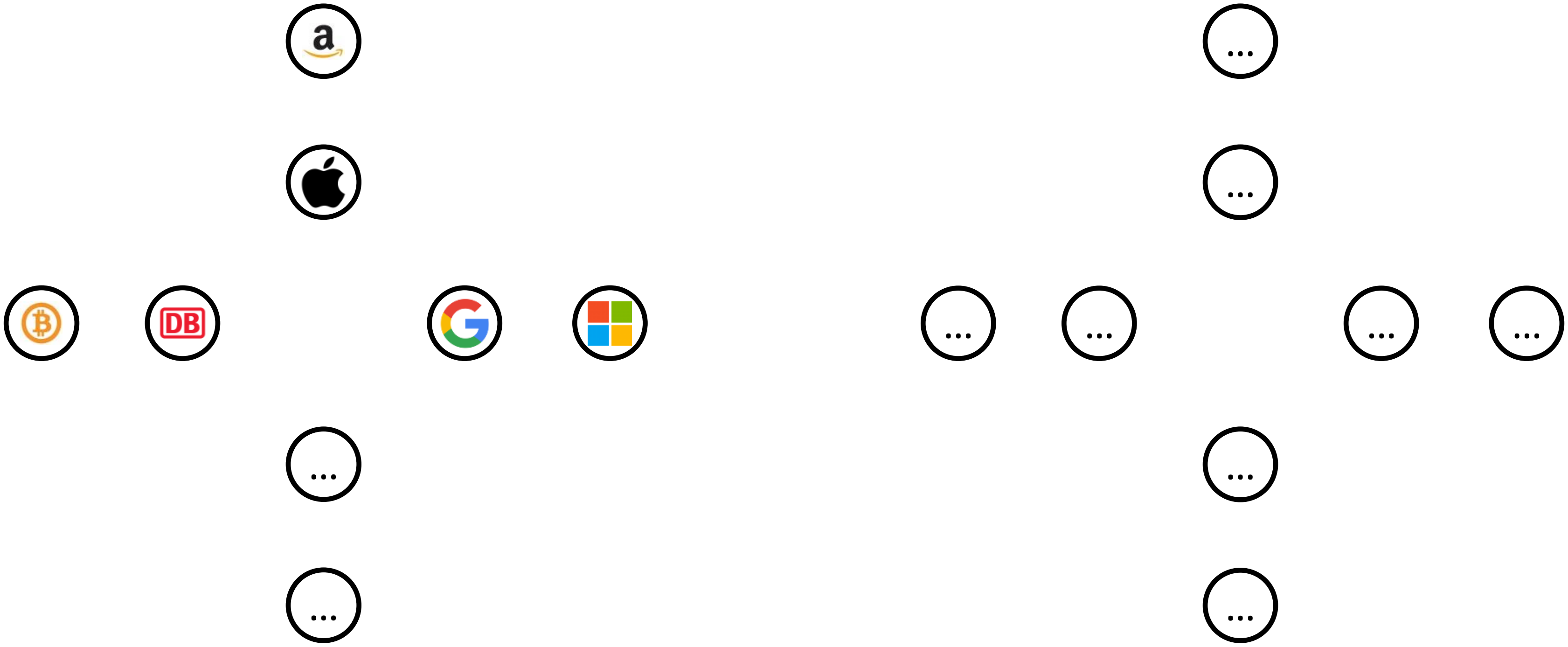
Spend budget, minimize risk, maximize outcome

Portfolio Optimization

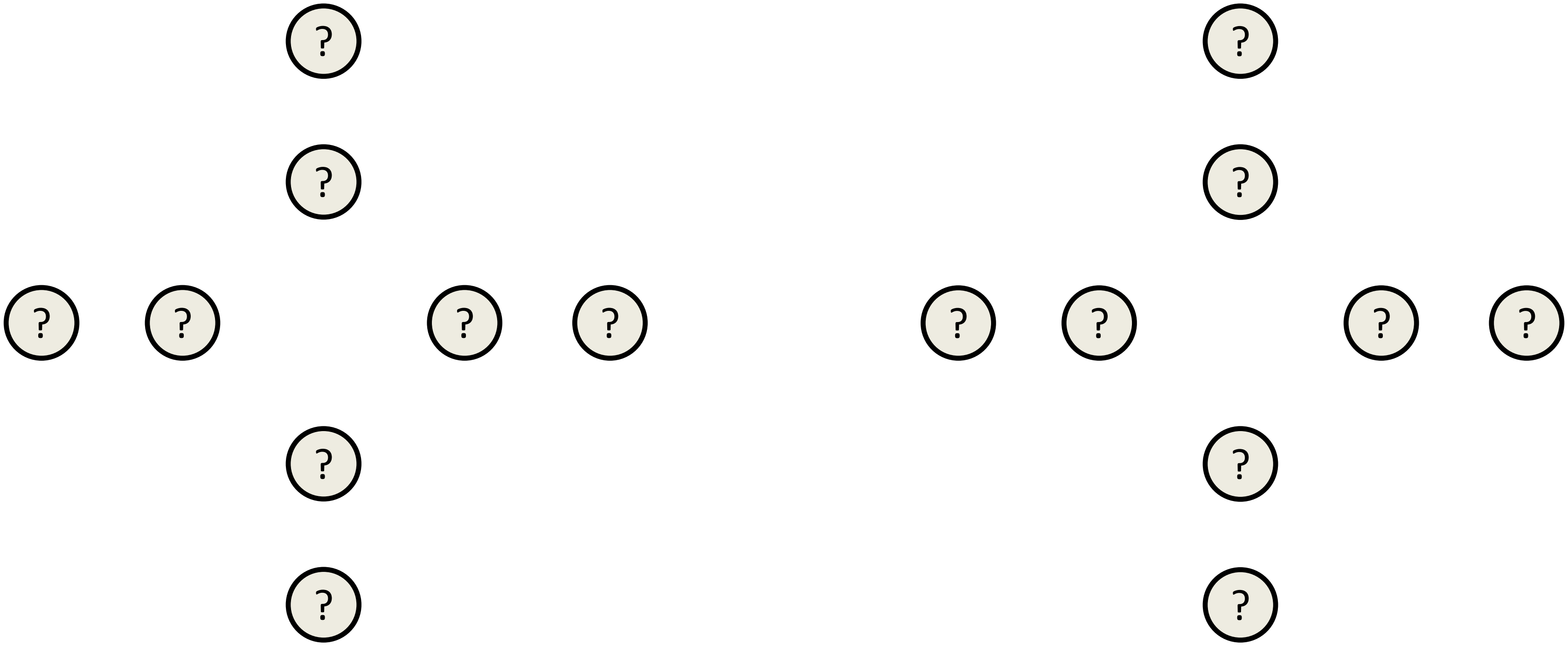
					…	
Buy			Buy	Buy	…	

Spend budget, minimize risk, maximize outcome

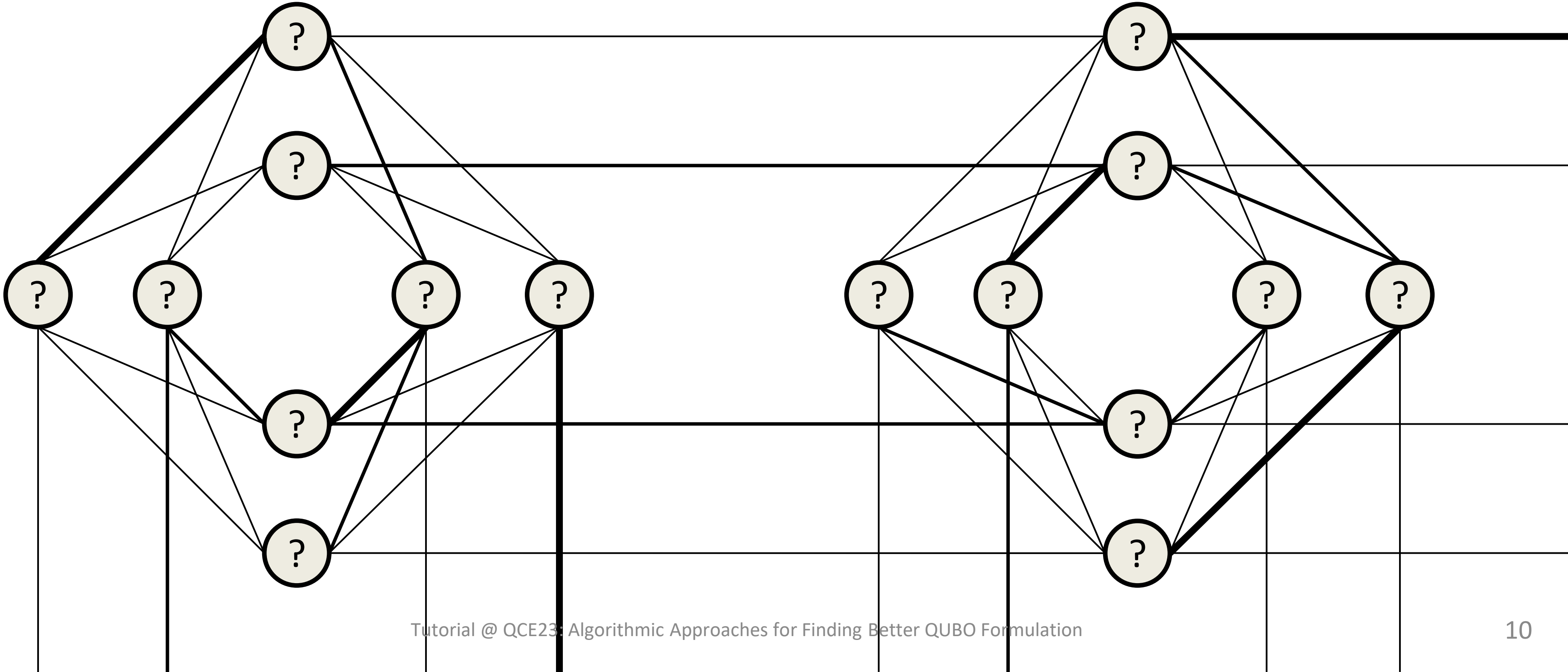
Qubits represent stocks



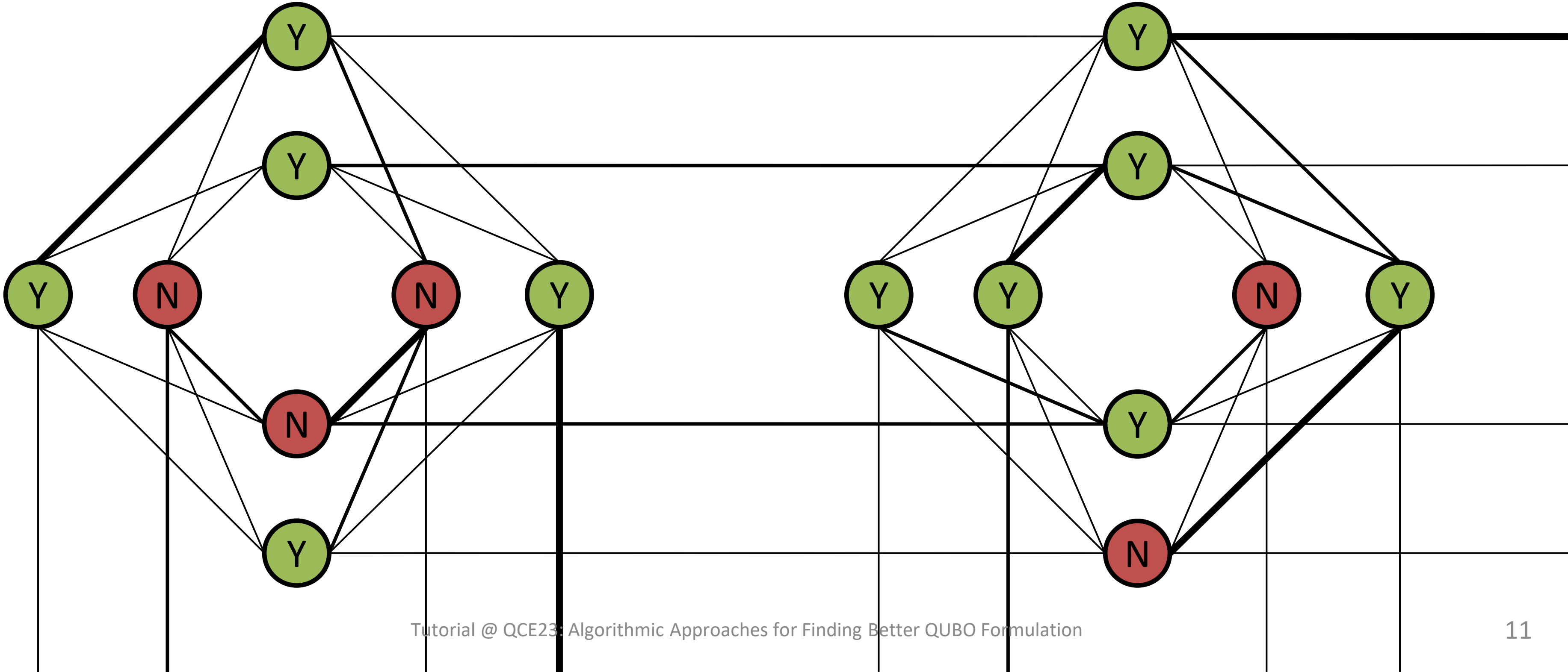
Initialize qubits in superposition



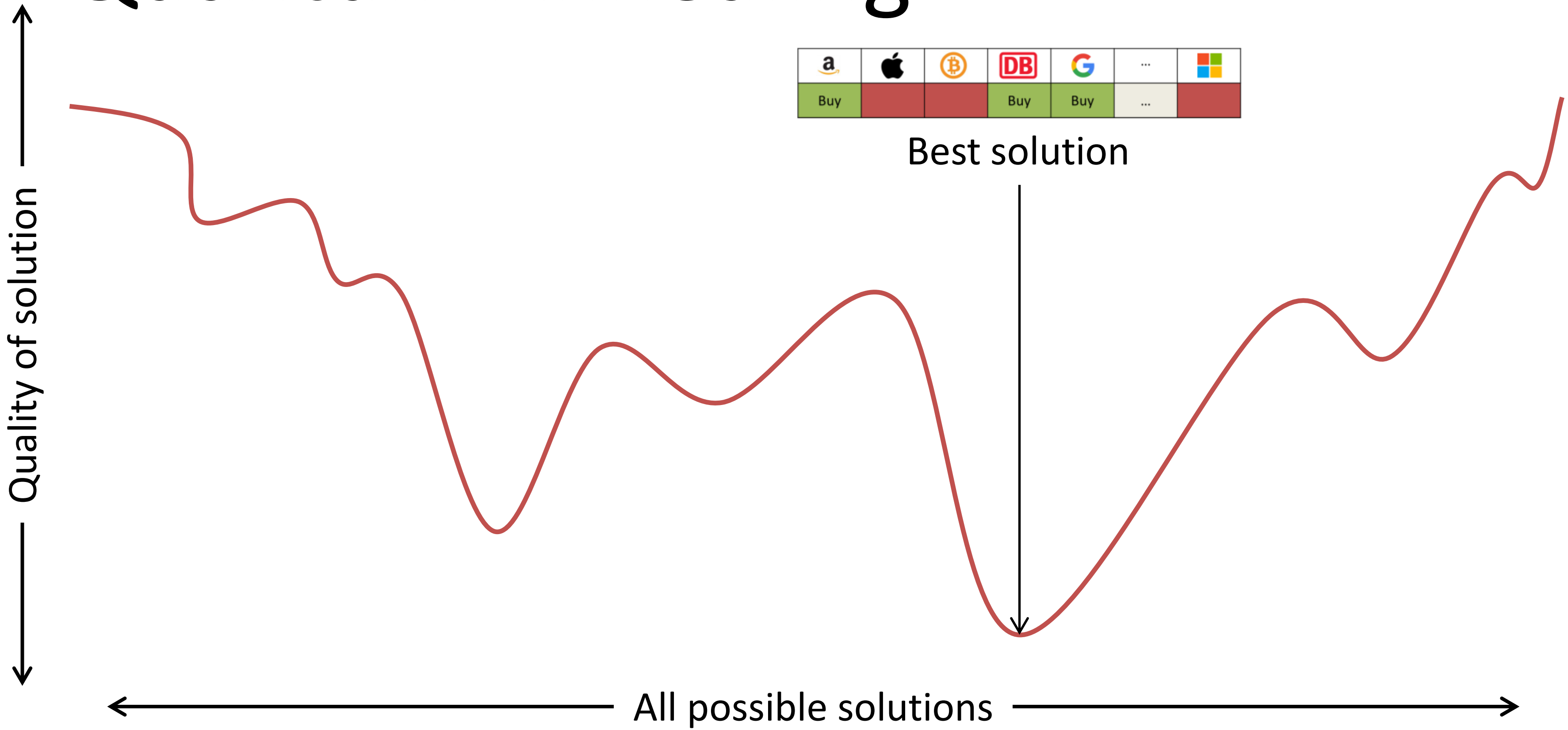
Formulate constraints

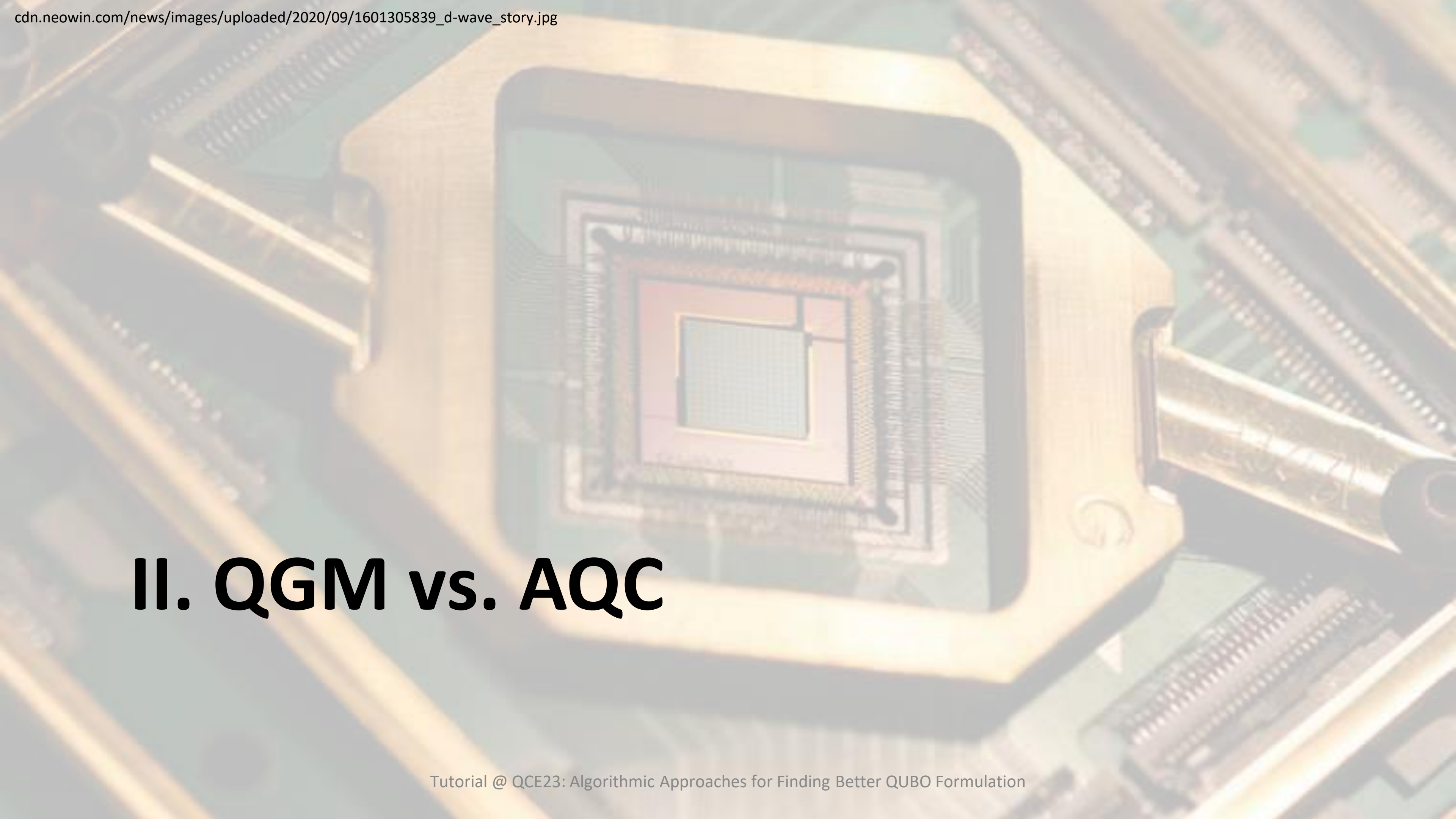


Anneal to optimal solution



Quantum Annealing





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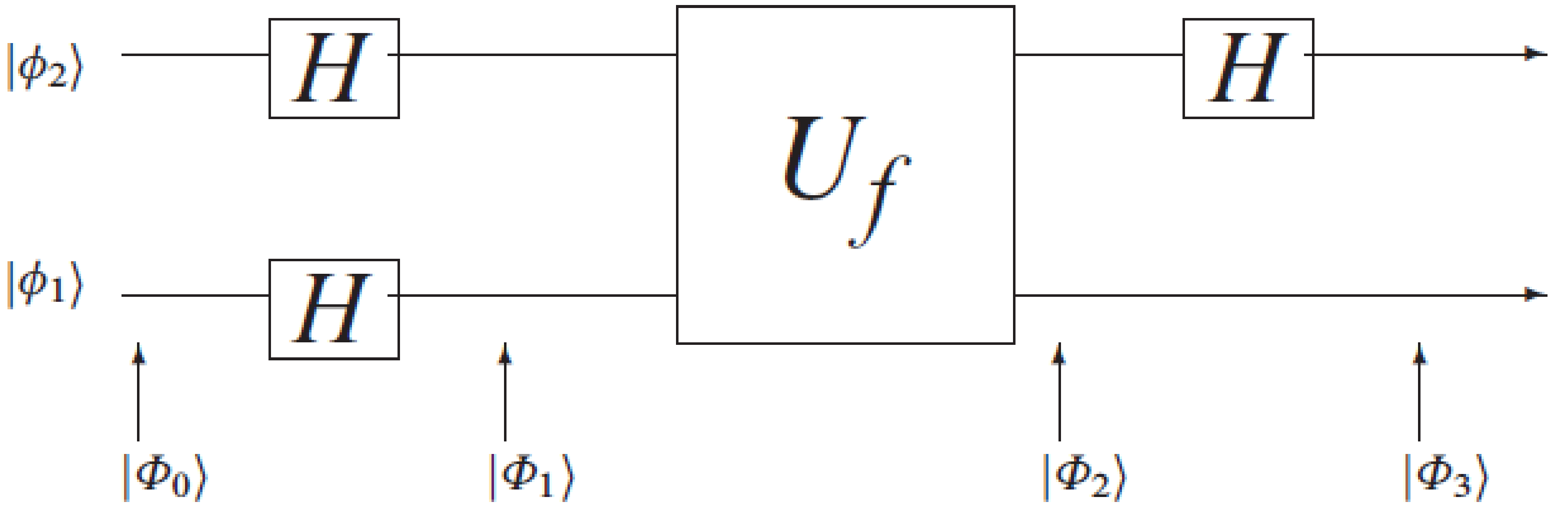
II. QGM vs. AQC

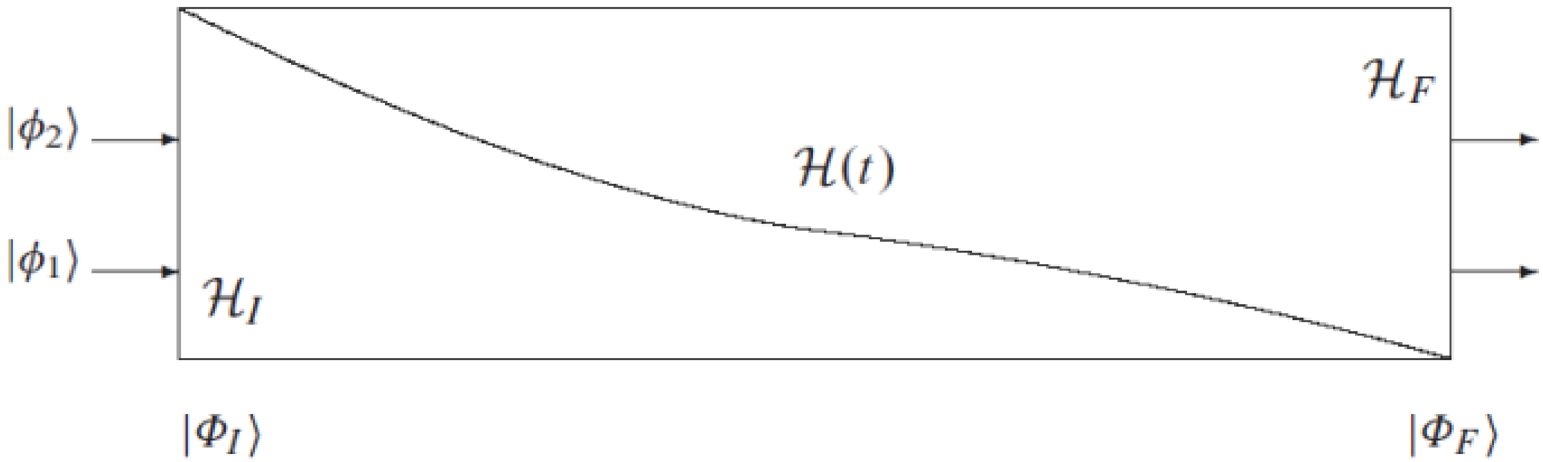
Source: McGeoch

Quantum Gate Model



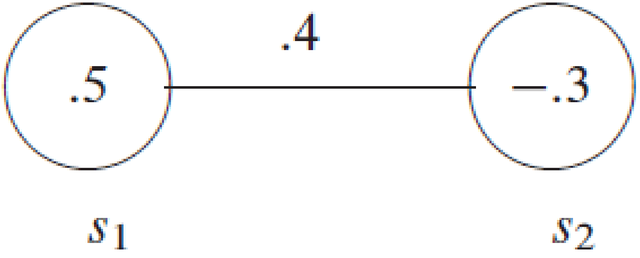
Source: McGeoch

Adiabatic Quantum Computation



Ising Model

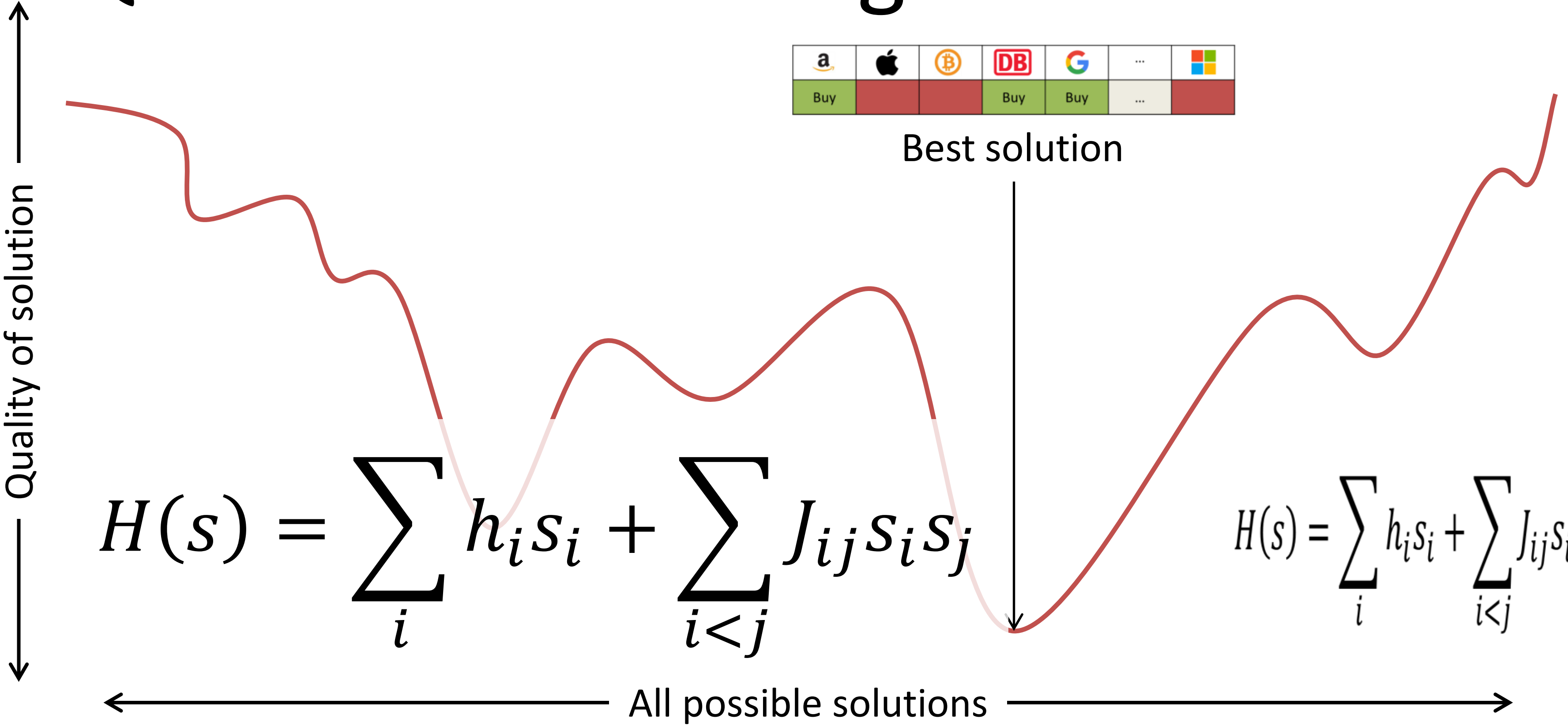
$$H(s) = \sum_{i} h_i s_i + \sum_{i<j} J_{ij} s_i s_j$$



Source: McGeoch

Quantum Annealing

a			DB	G	...	
Buy			Buy	Buy	...	



$$H(s) = \sum_{i} h_i s_i + \sum_{i<j} J_{ij} s_i s_j$$

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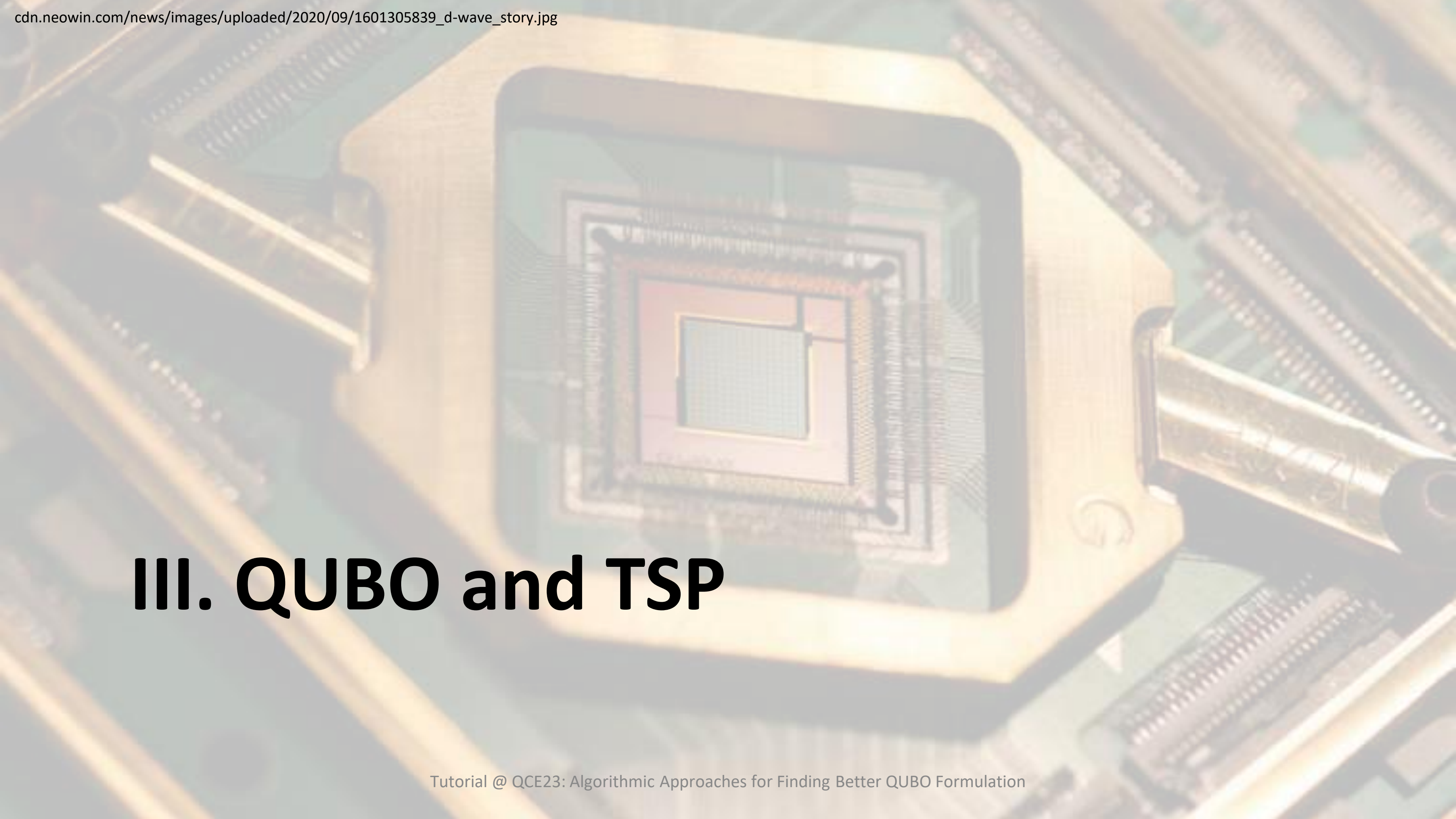
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III. QUBO and TSP

QUBO

Ising Model

$$H(s) = \sum_{i} h_i s_i + \sum_{i<j} J_{ij} s_i s_j$$

Quadratic Unconstrained Binary Optimization

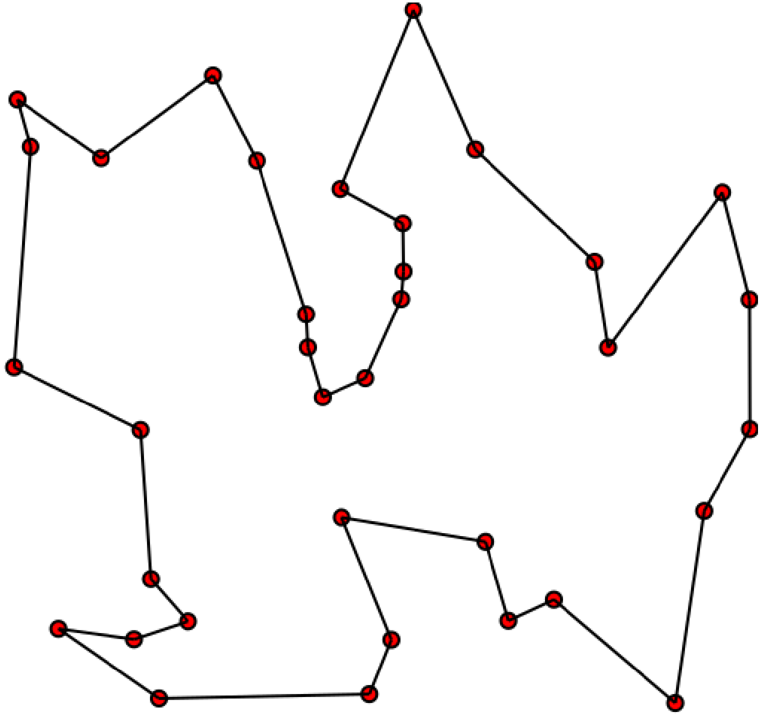
$$\sum_{i=1}^{N} c_i X_i + \sum_{i=1}^{N} \sum_{j=1}^{i} Q_{ij} X_i X_j$$

$$X_i \in \{0,1\}$$

$$c_i, Q_{ij} \in \mathbb{R}$$

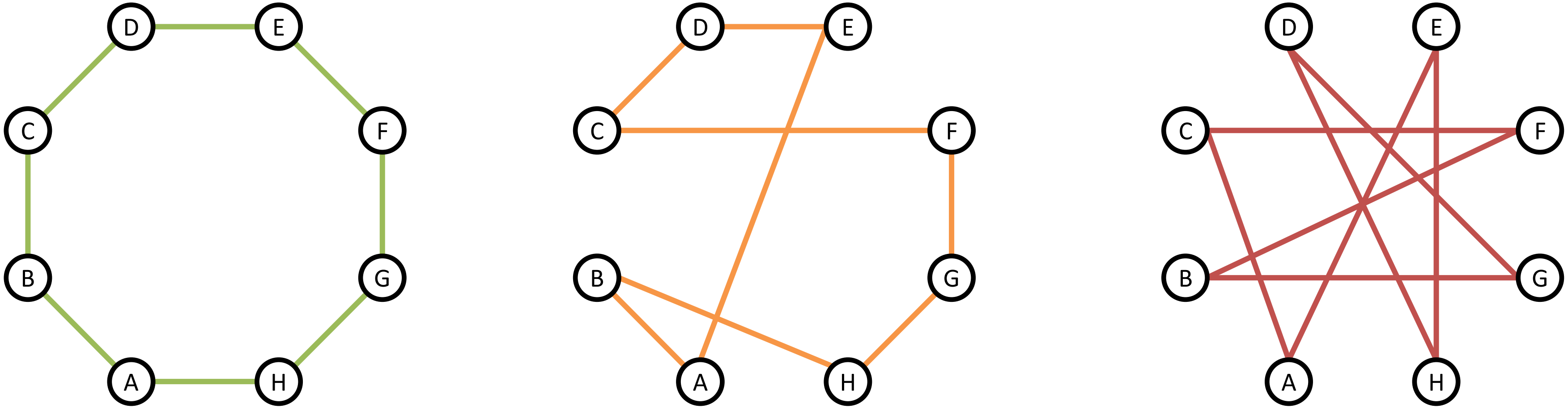
Source: Wikipedia

Travelling Salesman Problem



Given a list of cities and the distances between each pair of cities,
what is the shortest possible route that visits each city exactly once and returns to the origin city?

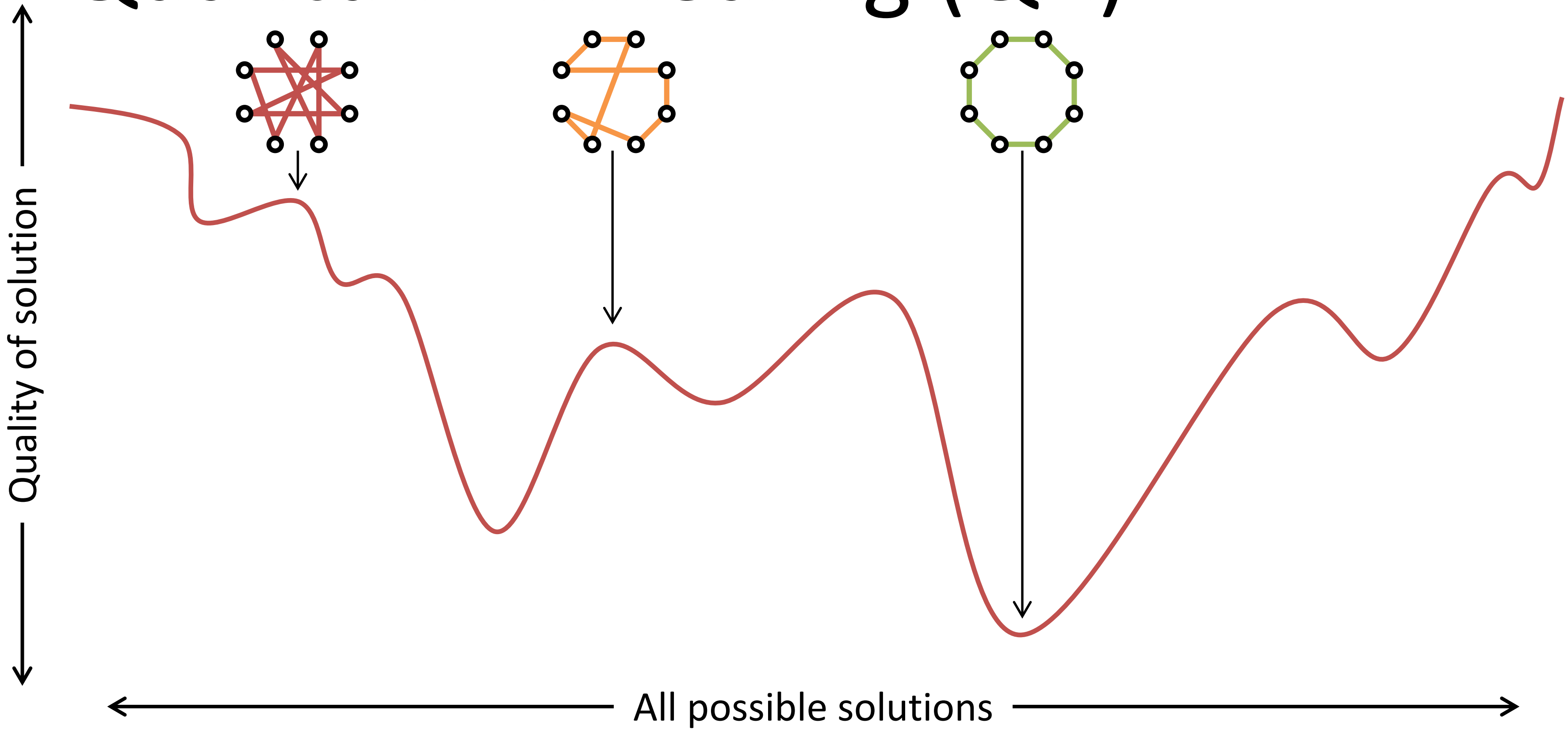
The Good, the Bad and the Ugly



Combinatorial Optimization

n cities	$(n-1)!$ combinations
2	1
3	2
4	6
5	24
10	362,880
20	1.2×10^{17}
100	9.3×10^{155}

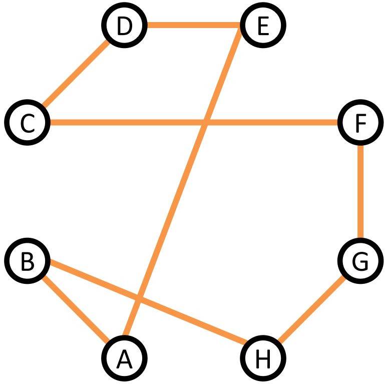
Quantum Annealing (QA)



Source: http://arxiv.org/pdf/1302.5843.pdf

TSP as Ising Formulation

$$H = \alpha \sum_{v=1}^{n} \left(1 - \sum_{j=1}^{N} x_{v,j}\right)^2 + \alpha \sum_{j=1}^{n} \left(1 - \sum_{v=1}^{N} x_{v,j}\right)^2 + \sum_{(uv)\in E} W_{uv} \sum_{j=1}^{N} x_{u,j} x_{v,j+1}$$

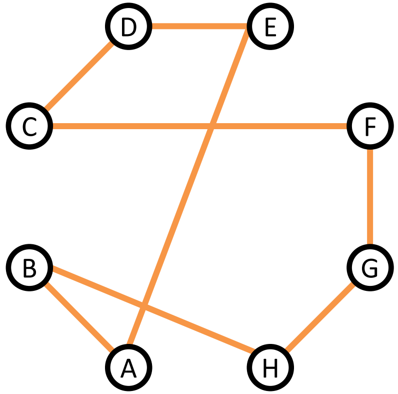


Given graph $G = (V, E)$ with edge weights W_{uv},

find hamiltonian cycle with minimum sum of edge weights

TSP as Ising Formulation

$$H = \alpha \sum_{v=1}^{n} \left(1 - \sum_{j=1}^{N} x_{v,j} \right)^2 + \alpha \sum_{j=1}^{n} \left(1 - \sum_{v=1}^{N} x_{v,j} \right)^2 + \sum_{(uv)\in E} W_{uv} \sum_{j=1}^{N} x_{u,j} x_{v,j+1}$$



	A1	A2	A3	A4	B1	B2	B3	B4	C1	C2	C3	C4
A1												
A2												
A3												
A4												
B1												
B2												
B3												
B4												

TSP as Ising Formulation

$$H = \alpha \sum_{v=1}^{n} \left(1 - \sum_{j=1}^{N} x_{v,j}\right)^2 + \alpha \sum_{j=1}^{n} \left(1 - \sum_{v=1}^{N} x_{v,j}\right)^2 + \sum_{(uv)\in E} W_{uv} \sum_{j=1}^{N} x_{u,j} x_{v,j+1}$$

	A1	A2	A3	A4	B1	B2	B3	B4	C1	C2	C3	C4
A1		α	α	α								
A2			α	α								
A3				α								
A4												
B1						α	α	α				
B2							α	α				
B3								α				
B4												

Every vertex can only appear once in a circle

TSP as Ising Formulation

$$H = \alpha \sum_{v=1}^{n} \left(1 - \sum_{j=1}^{N} x_{v,j}\right)^2 + \alpha \sum_{j=1}^{n} \left(1 - \sum_{v=1}^{N} x_{v,j}\right)^2 + \sum_{(uv)\in E} W_{uv} \sum_{j=1}^{N} x_{u,j} x_{v,j+1}$$

	A1	A2	A3	A4	B1	B2	B3	B4	C1	C2	C3	C4
A1		α	α	α	α				α			
A2			α	α		α				α		
A3				α			α				α	
A4								α				α
B1						α	α	α	α			
B2							α	α		α		
B3								α			α	
B4												α

There must be a j^{th} node in the cycle for each j

TSP as Ising Formulation

$$H = \alpha \sum_{v=1}^{n} \left(1 - \sum_{j=1}^{N} x_{v,j}\right)^2 + \alpha \sum_{j=1}^{n} \left(1 - \sum_{v=1}^{N} x_{v,j}\right)^2 + \underline{\sum_{(uv)\in E} W_{uv} \sum_{j=1}^{N} x_{u,j} x_{v,j+1}}$$

	A1	A2	A3	A4	B1	B2	B3	B4	C1	C2	C3	C4
A1		α	α	α	α	(ab)		(ba)	α	(ac)		(ca)
A2			α	α	(ba)	α	(ab)		(ca)	α	(ac)	
A3				α		(ba)	α	(ab)		(ca)	α	(ac)
A4					(ab)		(ba)	α	(ac)		(ca)	α
B1						α	α	α	α	(bc)		(cb)
B2							α	α	(cb)	α	(bc)	
B3								α		(cb)	α	(bc)
B4									(bc)		(cb)	α

If the edge is part of the cycle, apply the edge weight

TSP as Ising Formulation

$$H = \alpha \sum_{v=1}^{n} \left(1 - \sum_{j=1}^{N} x_{v,j}\right)^2 + \alpha \sum_{j=1}^{n} \left(1 - \sum_{v=1}^{N} x_{v,j}\right)^2 + \sum_{(uv)\in E} W_{uv} \sum_{j=1}^{N} x_{u,j} x_{v,j+1}$$

	A1	A2	A3	A4	B1	B2	B3	B4	C1	C2	C3	C4
A1	β	α	α	α	α	(ab)		(ba)	α	(ac)		(ca)
A2		β	α	α	(ba)	α	(ab)		(ca)	α	(ac)	
A3			β	α		(ba)	α	(ab)		(ca)	α	(ac)
A4				β	(ab)		(ba)	α	(ac)		(ca)	α
B1					β	α	α	α	α	(bc)		(cb)
B2						β	α	α	(cb)	α	(bc)	
B3							β	α		(cb)	α	(bc)
B4								β	(bc)		(cb)	α

Reward setting a qubit to 1 with negative value in diagonal

TSP as Ising Formulation

$$H = \alpha \sum_{v=1}^{n} \left(1 - \sum_{j=1}^{N} x_{v,j} \right)^2 + \alpha \sum_{j=1}^{n} \left(1 - \sum_{v=1}^{N} x_{v,j} \right)^2 + \sum_{(uv)\in E} W_{uv} \sum_{j=1}^{N} x_{u,j} x_{v,j+1}$$

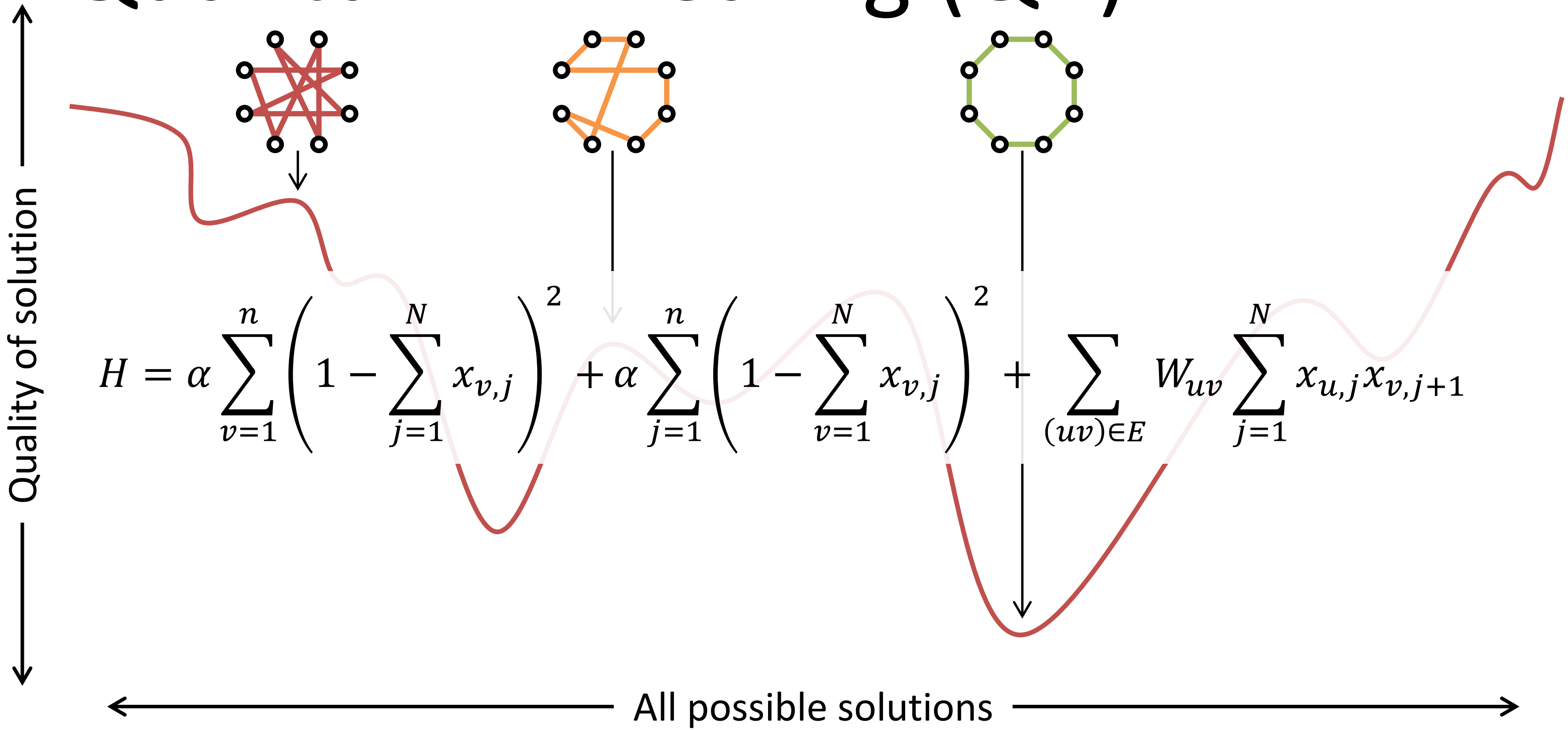
Every vertex can only appear once in a circle

There must be a j^{th} node in the cycle for each j

If the edge is part of the cycle, apply the edge weight

	A1	A2	A3	A4	B1	B2	B3	B4	C1	C2	C3	C4
A1	β	α	α	α	α	(ab)		(ba)	α	(ac)		(ca)
A2		β	α	α	(ba)	α	(ab)		(ca)	α	(ac)	
A3			β	α		(ba)	α	(ab)		(ca)	α	(ac)
A4				β	(ab)		(ba)	α	(ac)		(ca)	α
B1					β	α	α	α	α	(bc)		(cb)
B2						β	α	α	(cb)	α	(bc)	
B3							β	α		(cb)	α	(bc)
B4								β	(bc)		(cb)	α

Quantum Annealing (QA)



$$H = \alpha \sum_{v=1}^{n} \left(1 - \sum_{j=1}^{N} x_{v,j} \right)^2 + \alpha \sum_{j=1}^{n} \left(1 - \sum_{v=1}^{N} x_{v,j} \right)^2 + \sum_{(uv)\in E} W_{uv} \sum_{j=1}^{N} x_{u,j} x_{v,j+1}$$

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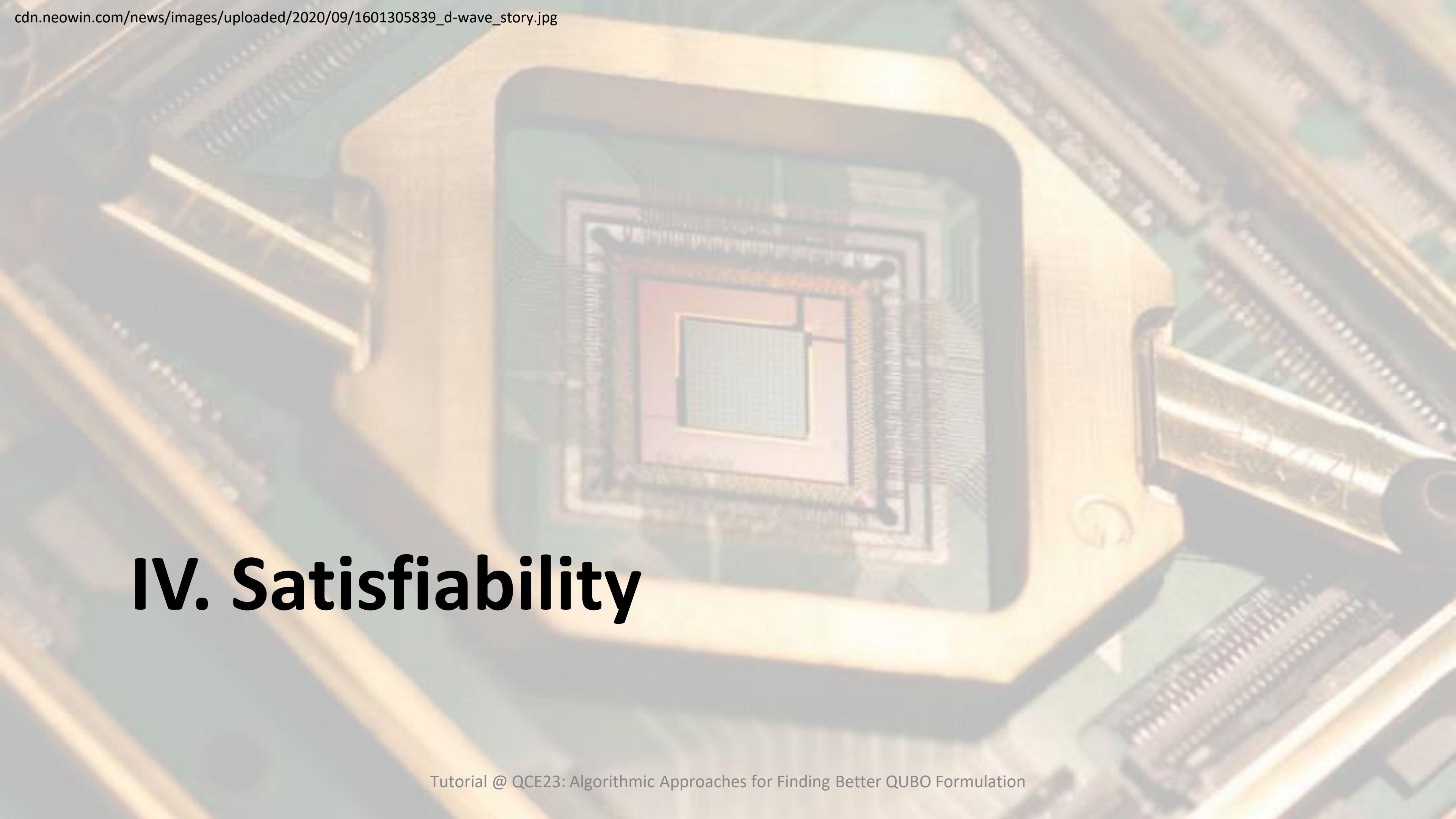
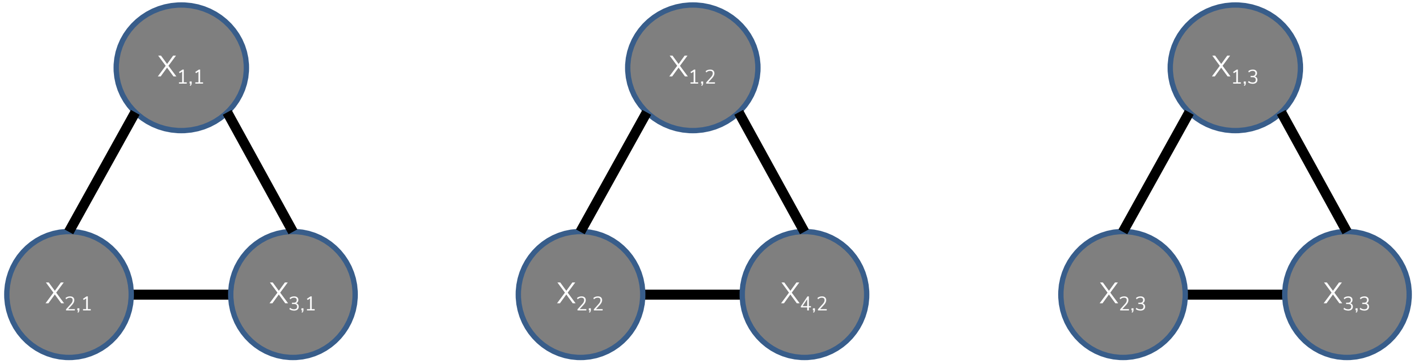


IV. Satisfiability

3SAT-to-QUBO transformation (Choi)

$$\Phi = (x_1 \vee x_2 \vee x_3) \wedge (-x_1 \vee x_2 \vee x_4) \wedge (x_1 \vee -x_2 \vee x_3)$$

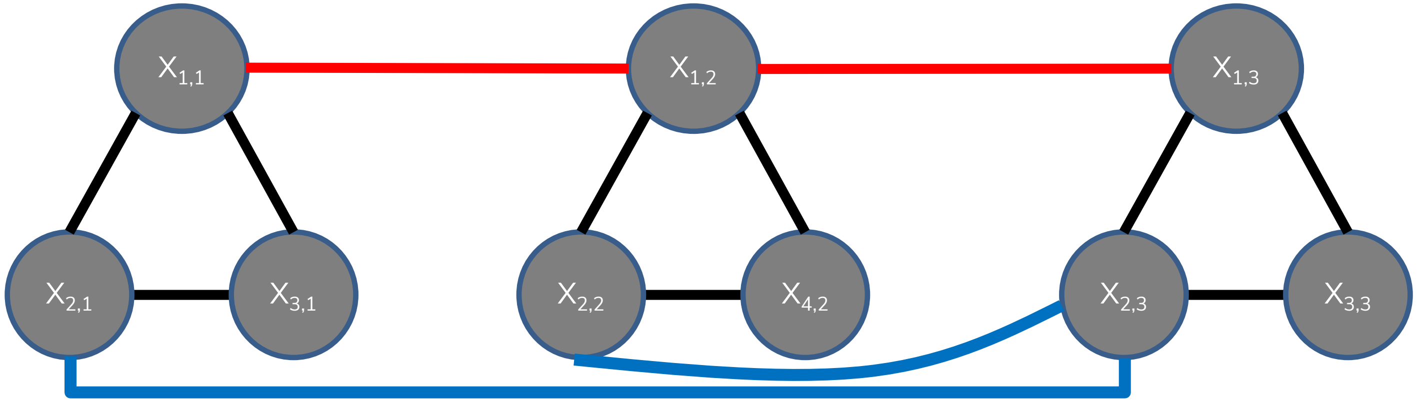
- Step 1: Build a graph structure for each clause



3SAT-to-QUBO transformation (Choi)

$$\Phi = (x_1 \vee x_2 \vee x_3) \wedge (-x_1 \vee x_2 \vee x_4) \wedge (x_1 \vee -x_2 \vee x_3)$$

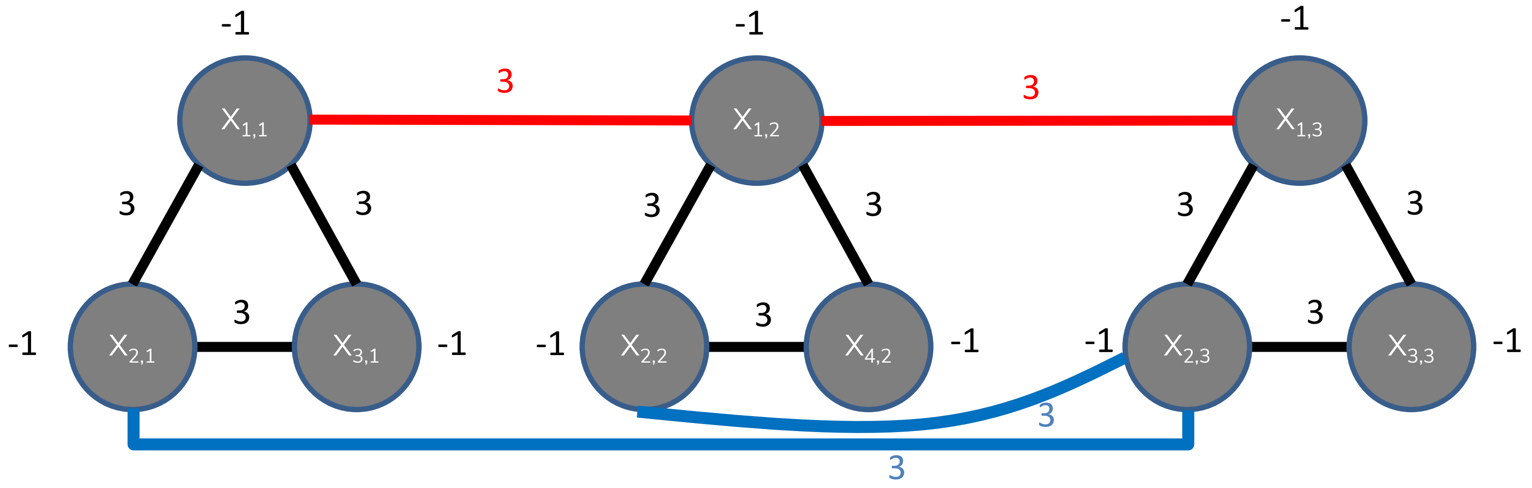
- Step 2: Interconnect conflicting literals from different clauses



3SAT-to-QUBO transformation (Choi)

$$\Phi = (x_1 \vee x_2 \vee x_3) \wedge (-x_1 \vee x_2 \vee x_4) \wedge (x_1 \vee -x_2 \vee x_3)$$

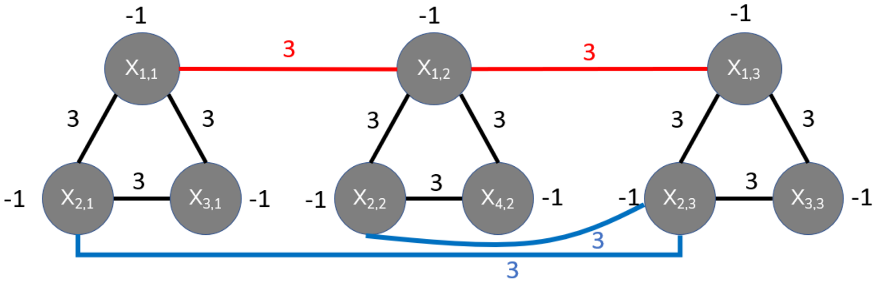
- Step 3: Add weights



3SAT-to-QUBO transformation (Choi)

$$\Phi = (x_1 \vee x_2 \vee x_3) \wedge (-x_1 \vee x_2 \vee x_4) \wedge (x_1 \vee -x_2 \vee x_3)$$

- Step 4: Rewrite as QUBO

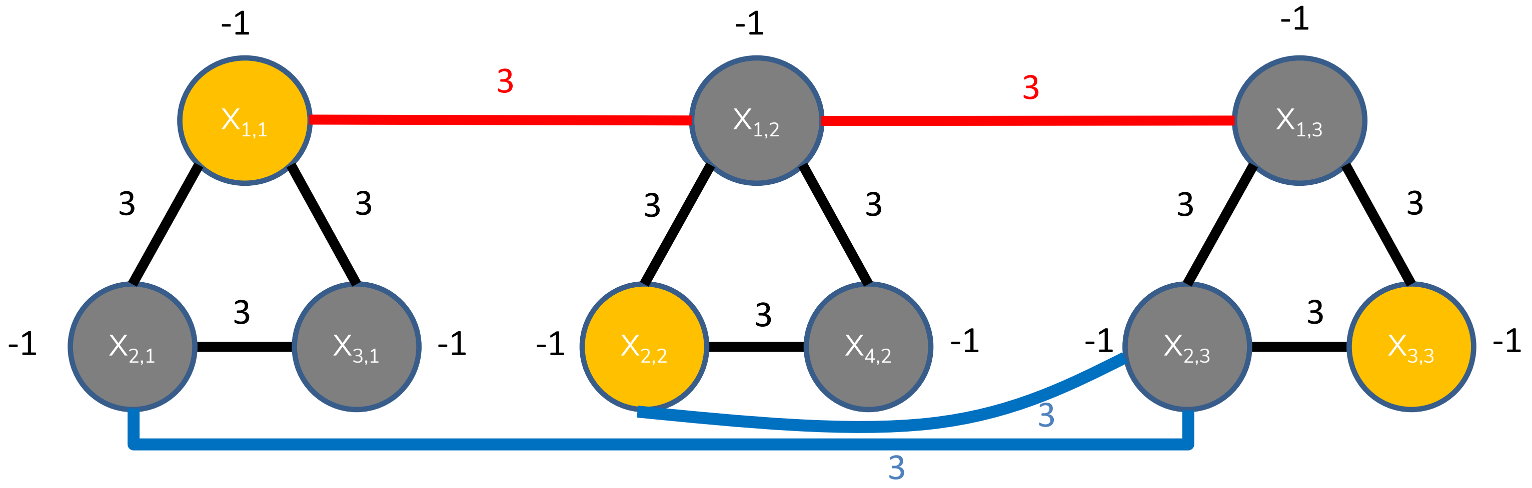


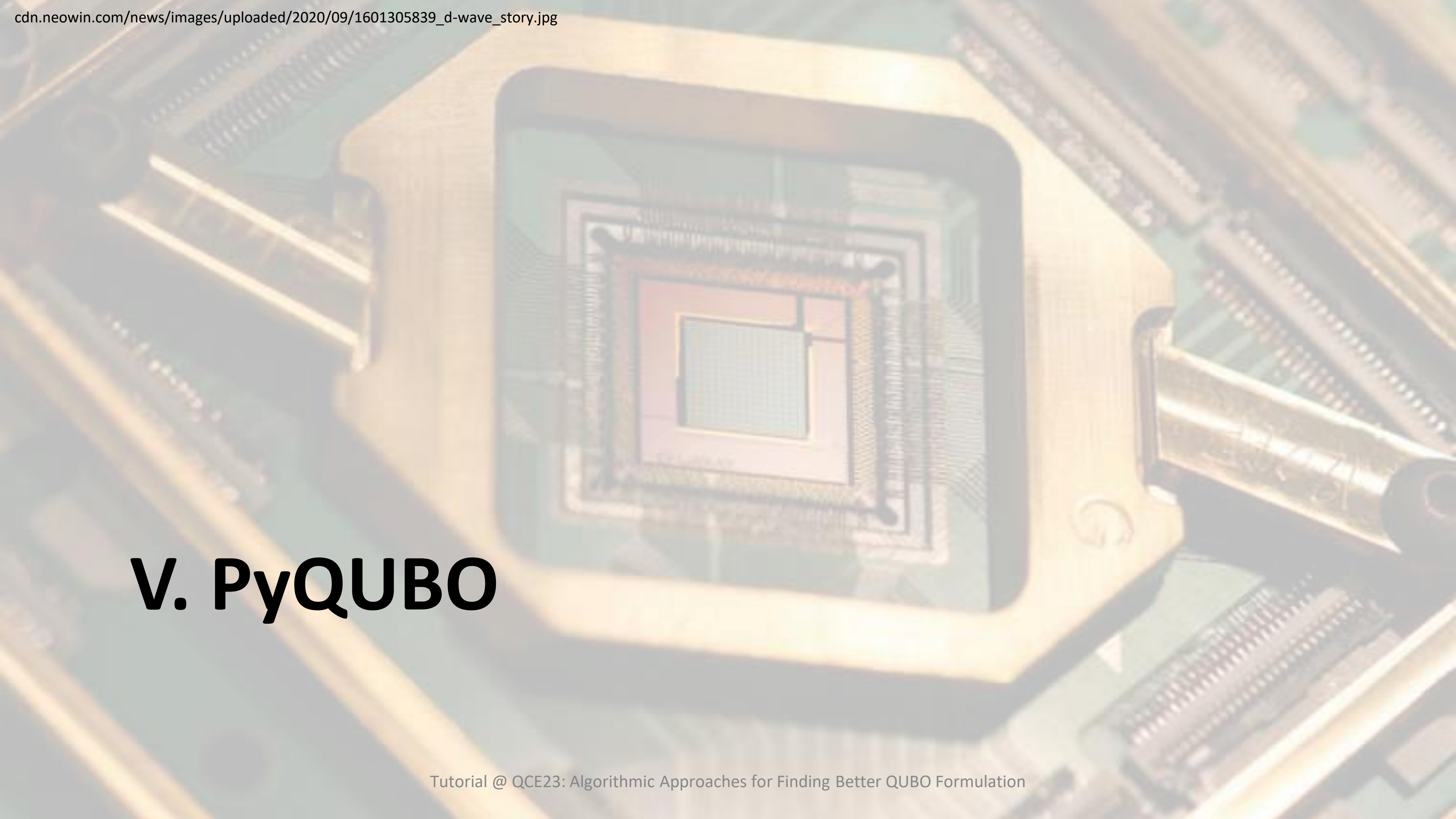
	$X_{1,1}$	$X_{2,1}$	$X_{3,1}$	$X_{1,2}$	$X_{2,2}$	$X_{4,2}$	$X_{1,3}$	$X_{2,3}$	$X_{3,3}$
$X_{1,1}$	-1	3	3	3					
$X_{2,1}$		-1	3					3	
$X_{3,1}$			-1						
$X_{1,2}$				-1	3	3	3		
$X_{2,2}$					-1	3		3	
$X_{4,2}$						-1			
$X_{1,3}$							-1	3	3
$X_{2,3}$								-1	3
$X_{3,3}$									-1

3SAT-to-QUBO transformation (Choi)

$$\Phi = (x_1 \vee x_2 \vee x_3) \wedge (-x_1 \vee x_2 \vee x_4) \wedge (x_1 \vee -x_2 \vee x_3)$$

- Solutions: Independent sets minimizing node sums





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V. PyQUBO

PyQUBO

- Open-source Python library for constructing QUBOs matrices from objective functions and constraints of optimization problems
- Features abstraction of expressions and extensibility of the program to create QUBO instances and Ising models
- Examples: number partitioning problem, knapsack problem, graph coloring problem, and integer factorization using a binary multiplier

IEEE Transactions on Computers

PyQUBO: Python Library for Mapping Combinatorial Optimization Problems to QUBO Form

April 2022, pp. 838-850, vol. 71
DOI Bookmark: 10.1109/TC.2021.3063618

Authors

Mashiyat Zaman, Recruit Co., Ltd., Chuo-ku, Tokyo, Japan
Kotaro Tanahashi, Recruit Co., Ltd., Chuo-ku, Tokyo, Japan
Shu Tanaka, Department of Applied Physics and Physico-Informatics, Keio University, Kanagawa, Japan

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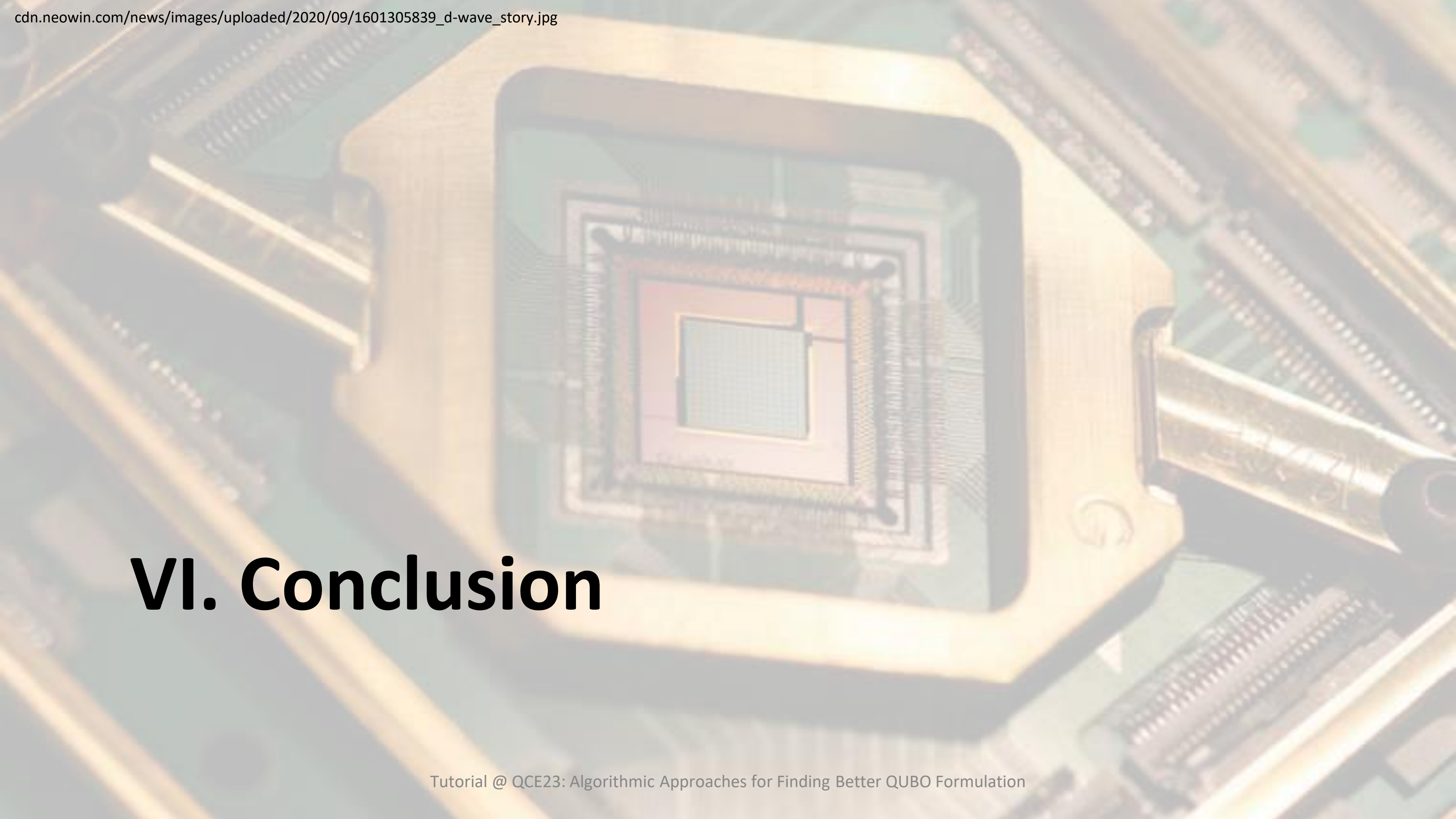

VI. Conclusion

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THE REAL WORLD $\xrightarrow{?}$

$$\sum_{i=1}^{N} c_i X_i + \sum_{i=1}^{N} \sum_{j=1}^{i} Q_{ij} X_i X_j$$

$$X_i \in \{0,1\}$$

$$c_i, Q_{ij} \in \mathbb{R}$$

Naïve QUBO Formulations

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Thank you!