

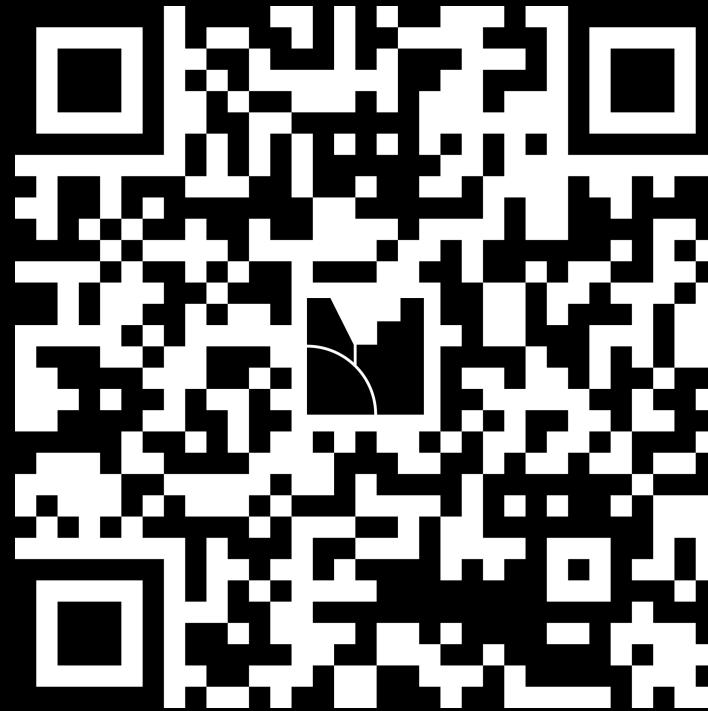


AI for Accelerated Quantum Supercomputing

Monica VanDieren, PhD | QC4MC August 12, 2025

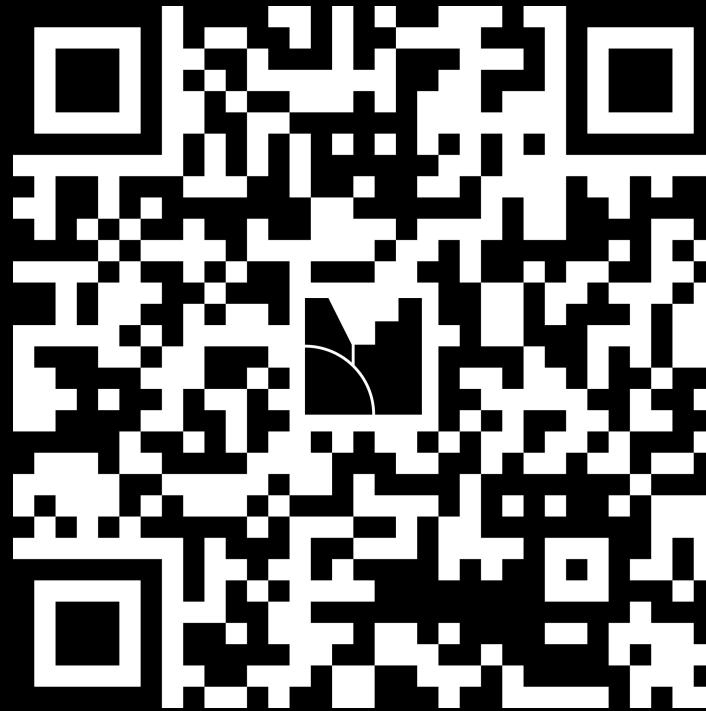
AI for Accelerated Quantum Computing

menti.com
Code:2569 6565



How familiar are you with ...?

menti.com
Code: 2569 6565



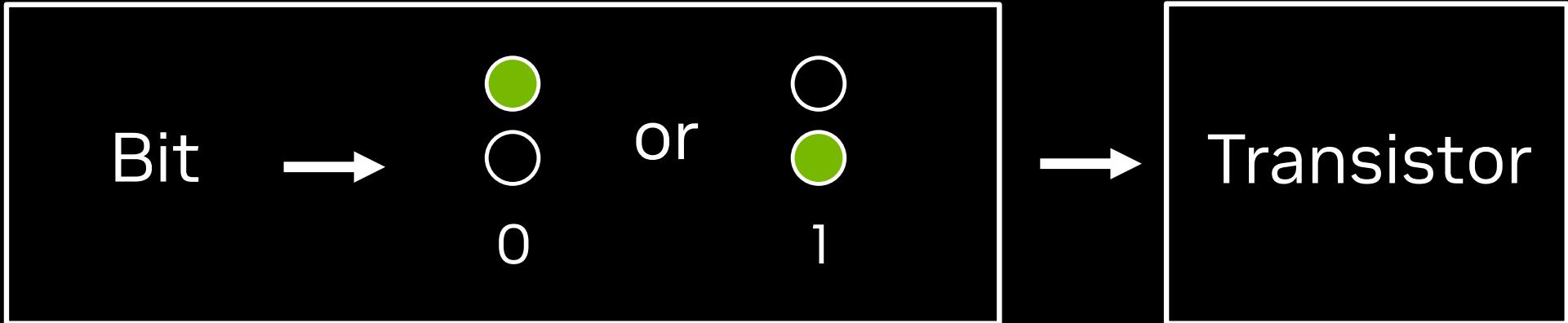


Agenda

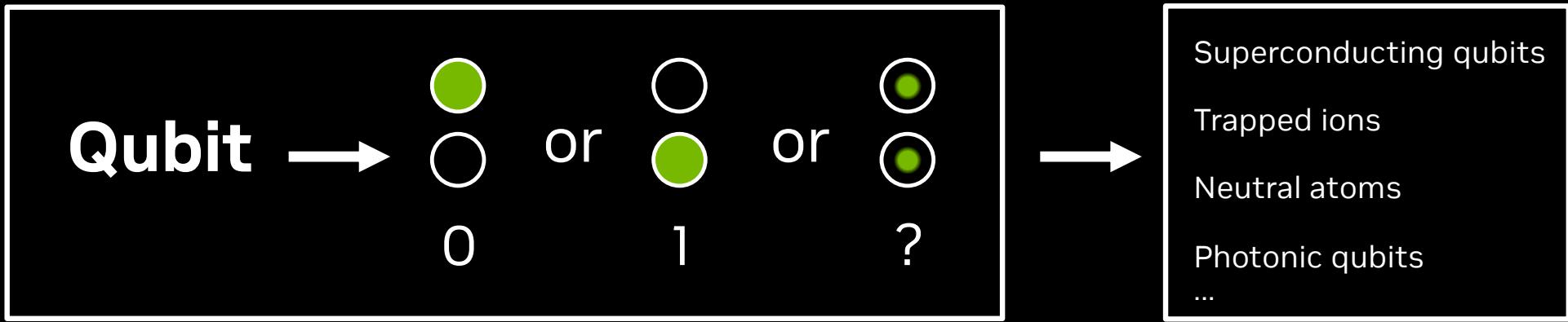
- Quantum circuits and quantum kernels
- AI for Accelerated Quantum Supercomputing
- Variational Algorithm and Adaptive Circuit Knitting
- Resources to learn more about Accelerated Quantum Supercomputing

What is a Quantum Computer?

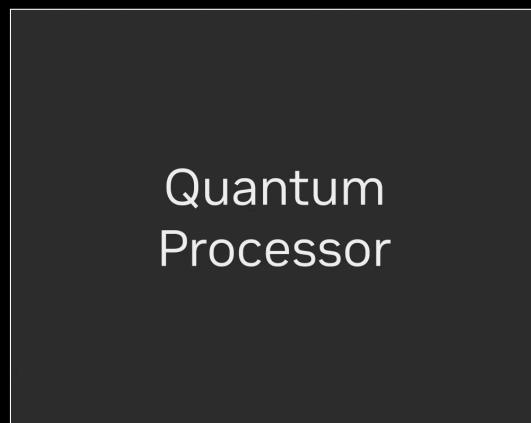
Conventional computer



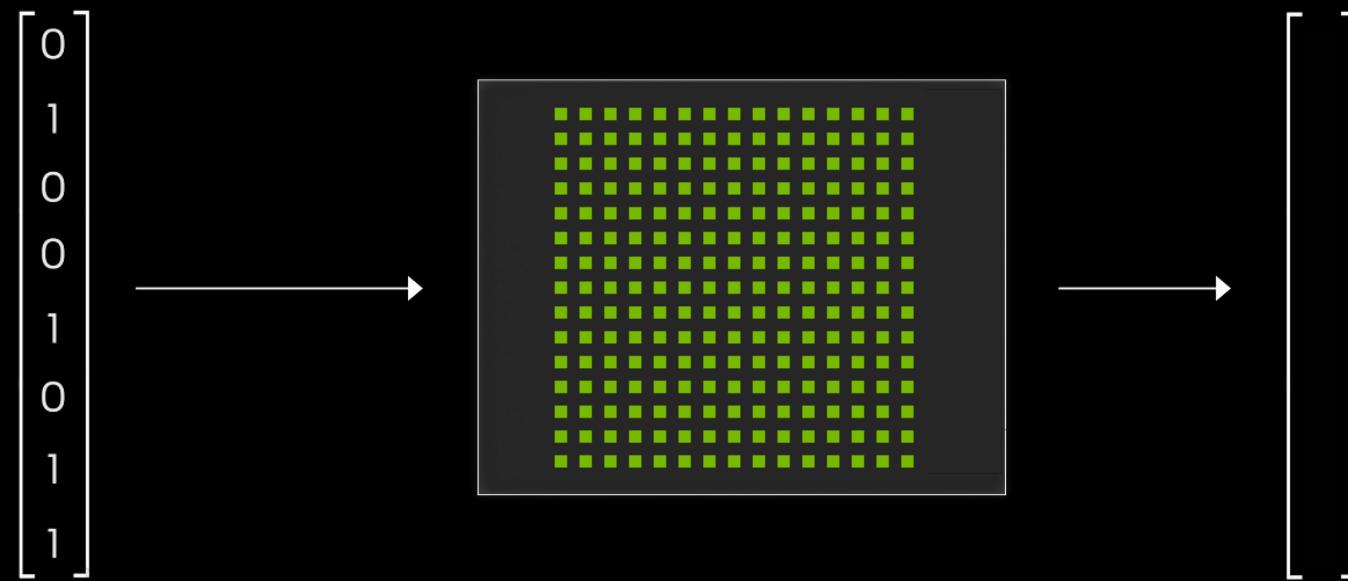
Quantum computer



$$\begin{bmatrix} 1 \\ 0 \\ 1 \\ 1 \\ 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}$$

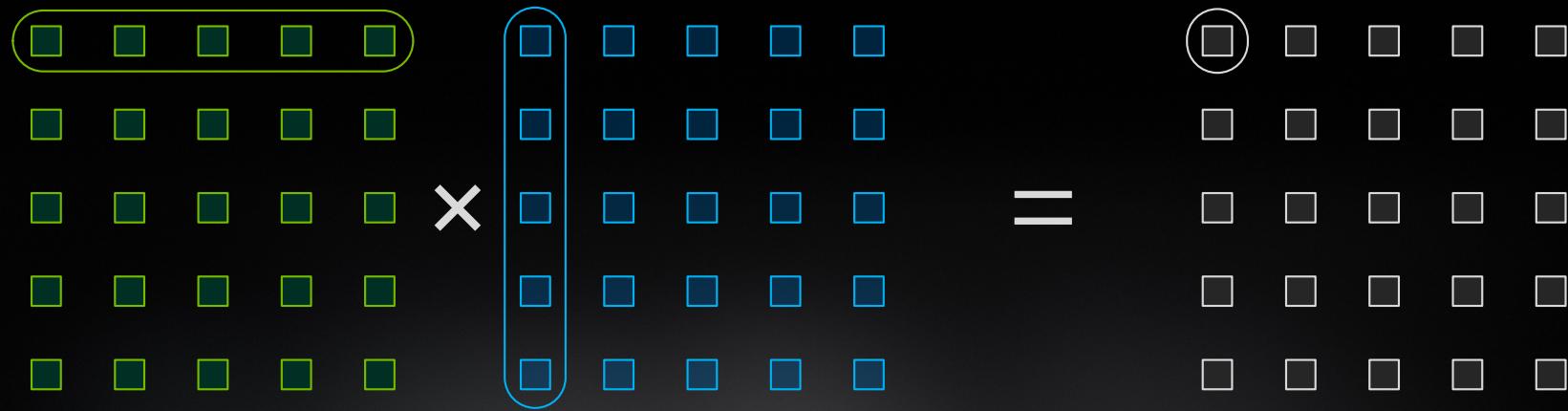


Matrix Multiplication

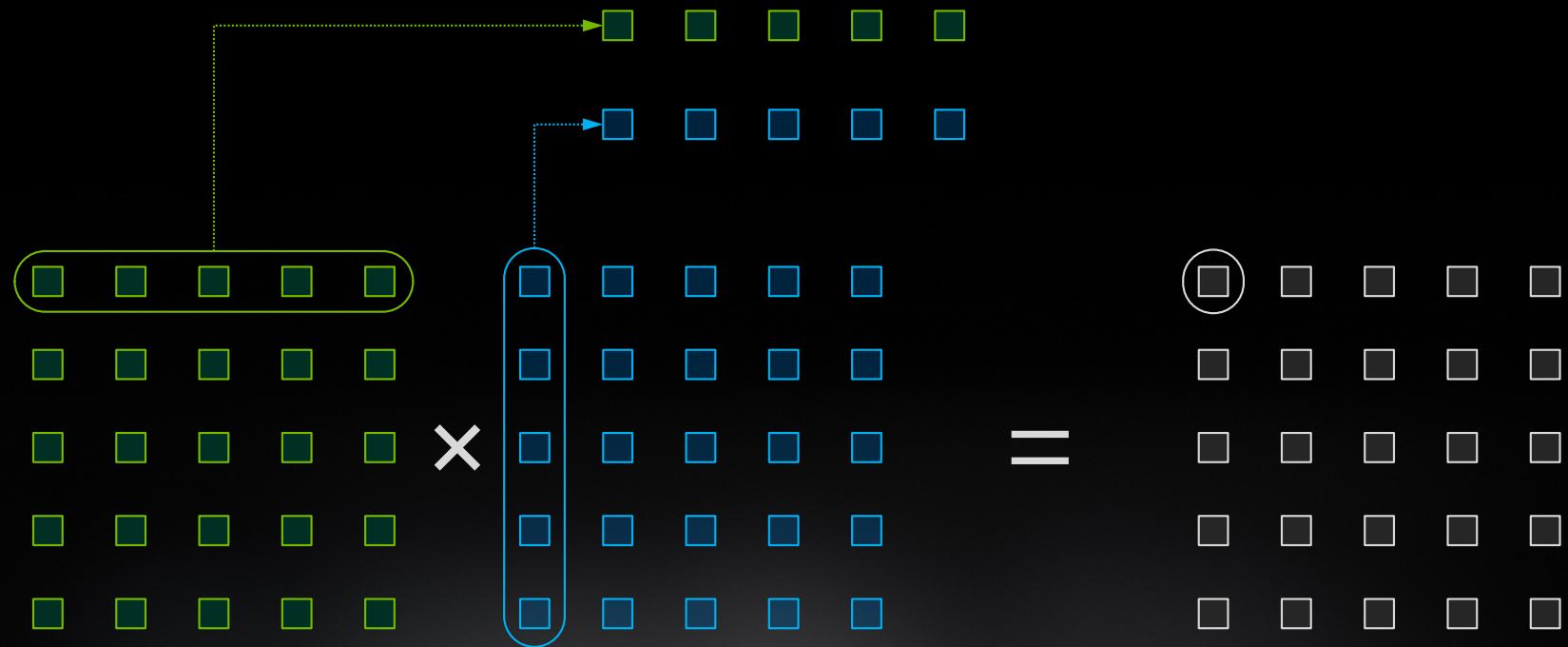


A quantum processor acting on N qubits
can be modeled by a $2^N \times 2^N$ matrix

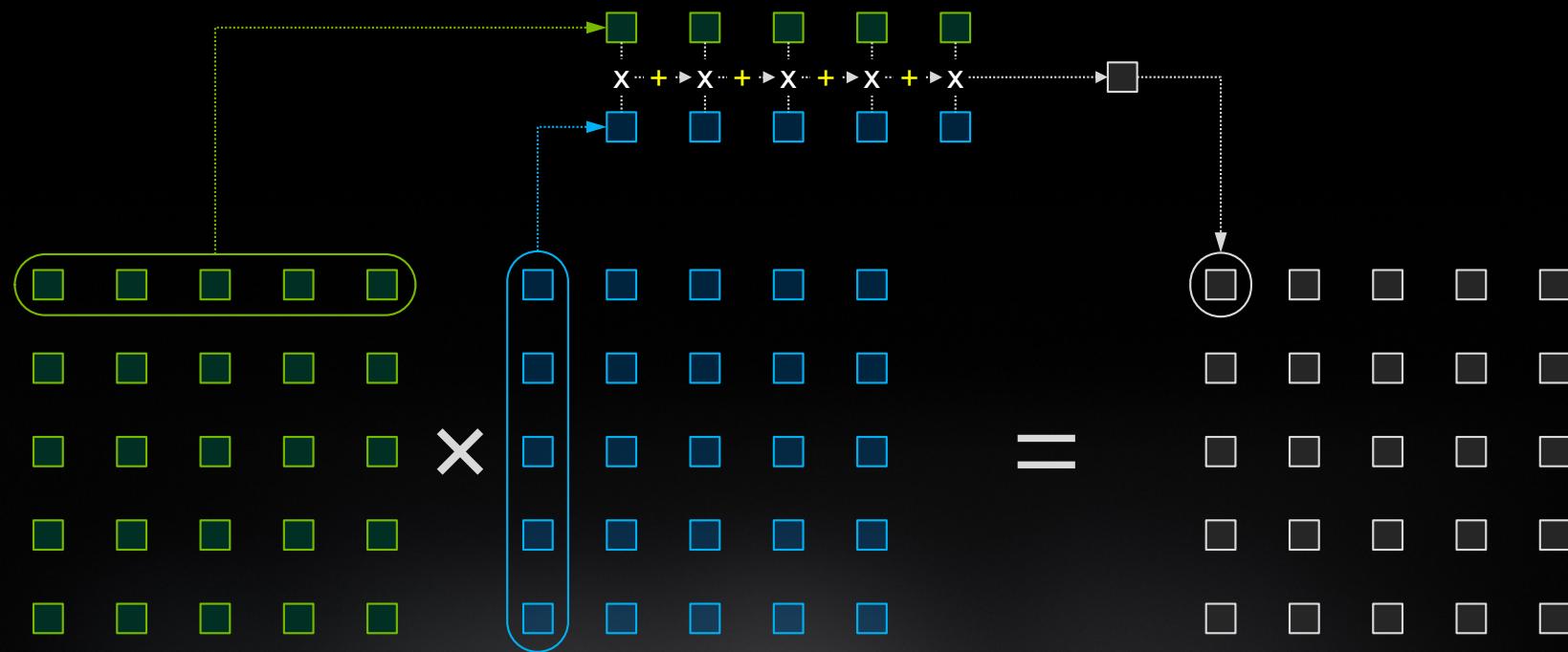
Matrix Multiplication



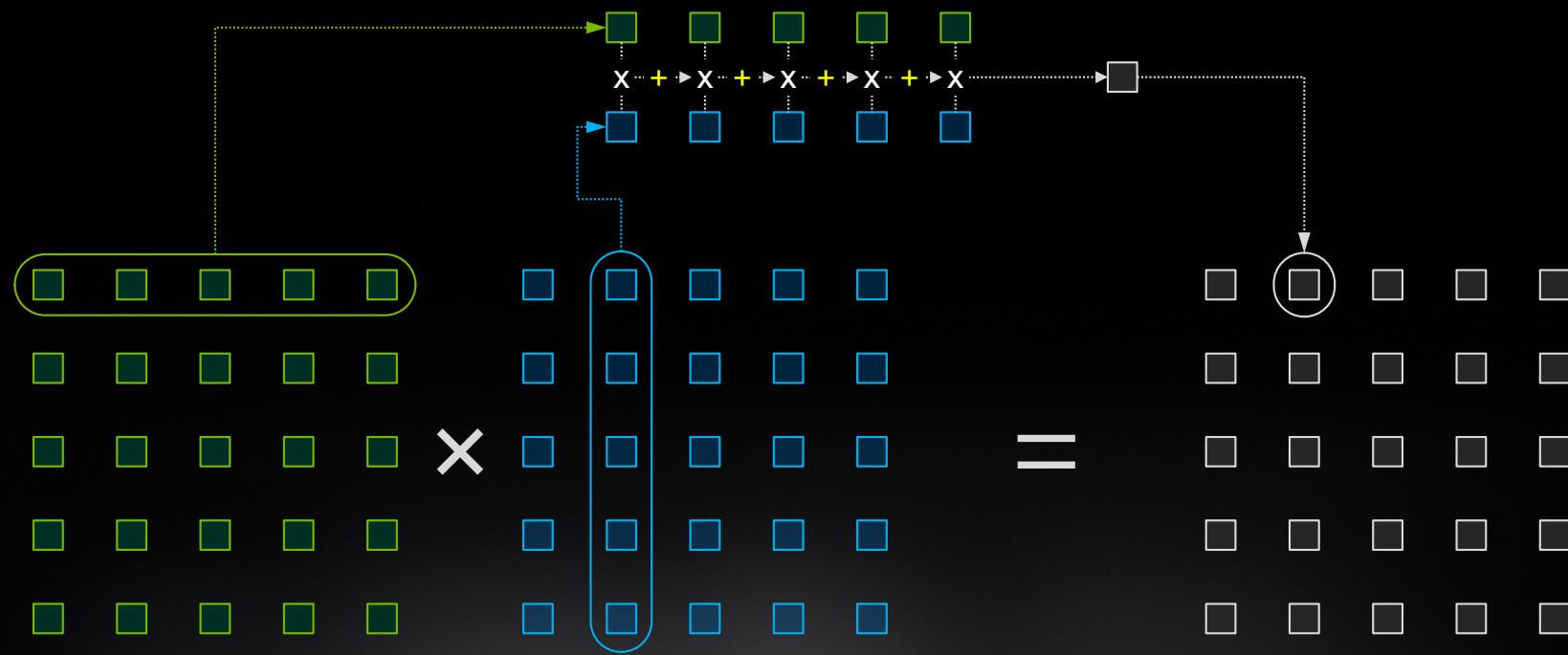
Matrix Multiplication



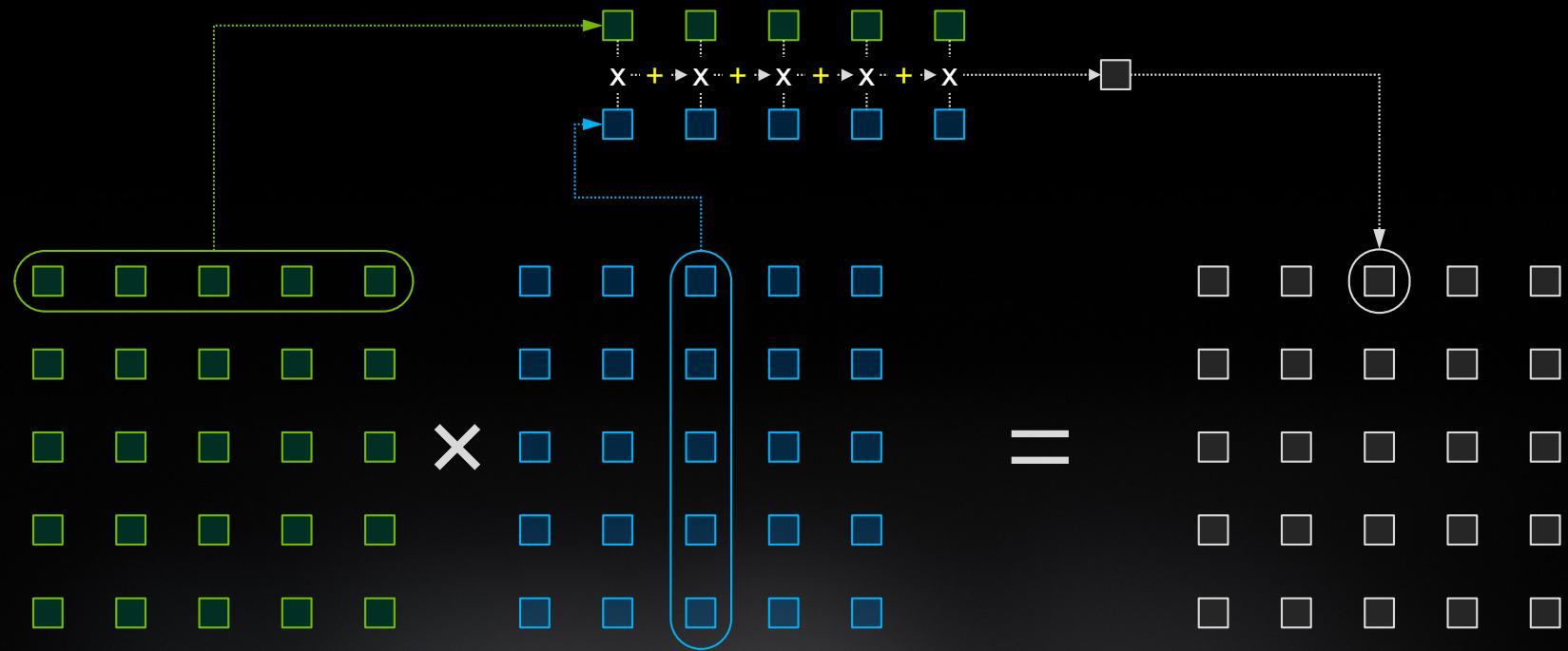
Matrix Multiplication



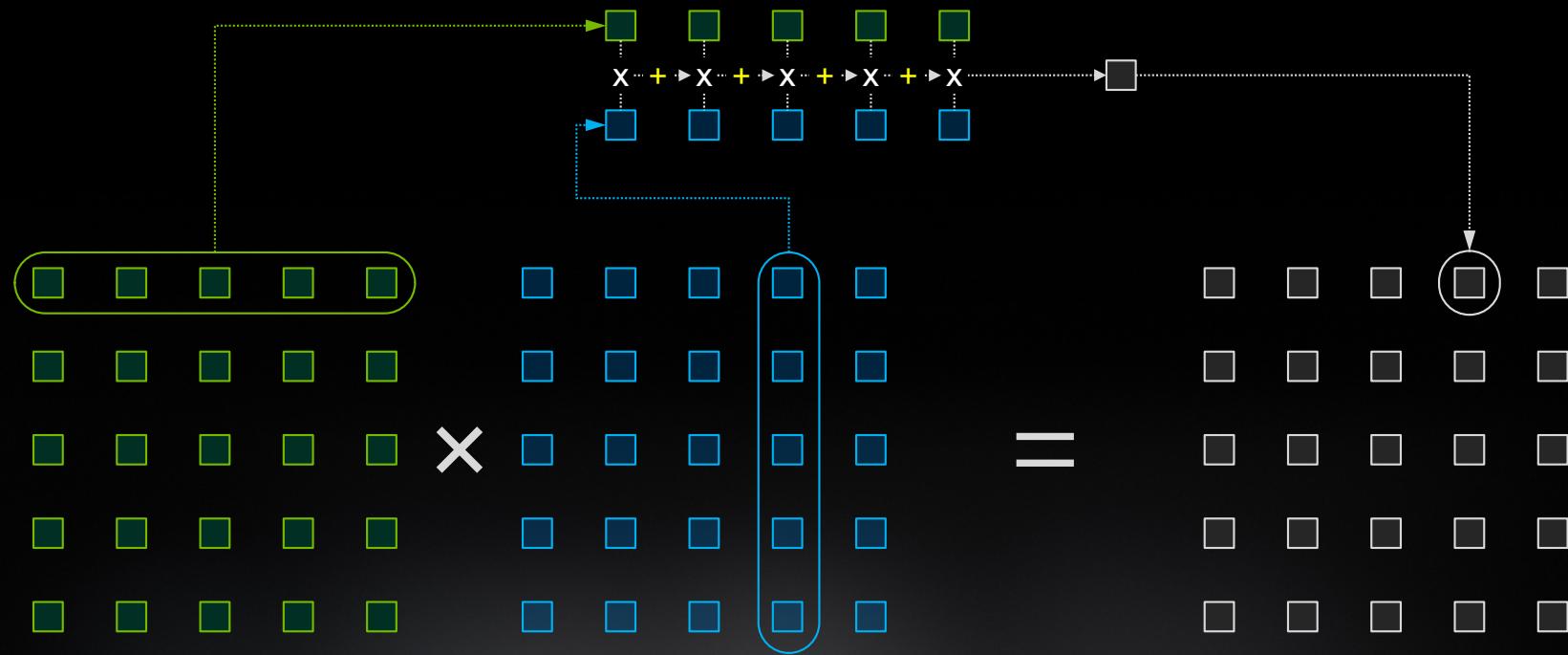
Matrix Multiplication



Matrix Multiplication

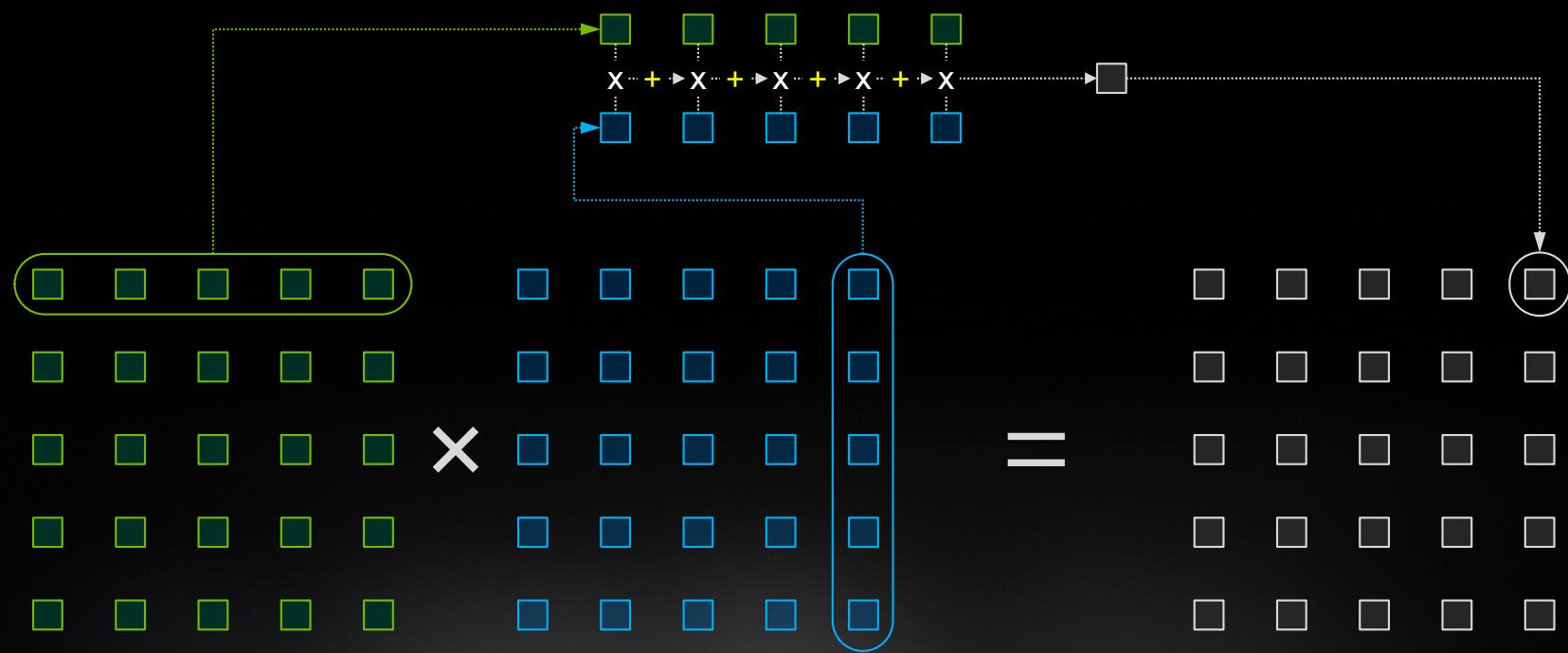


Matrix Multiplication



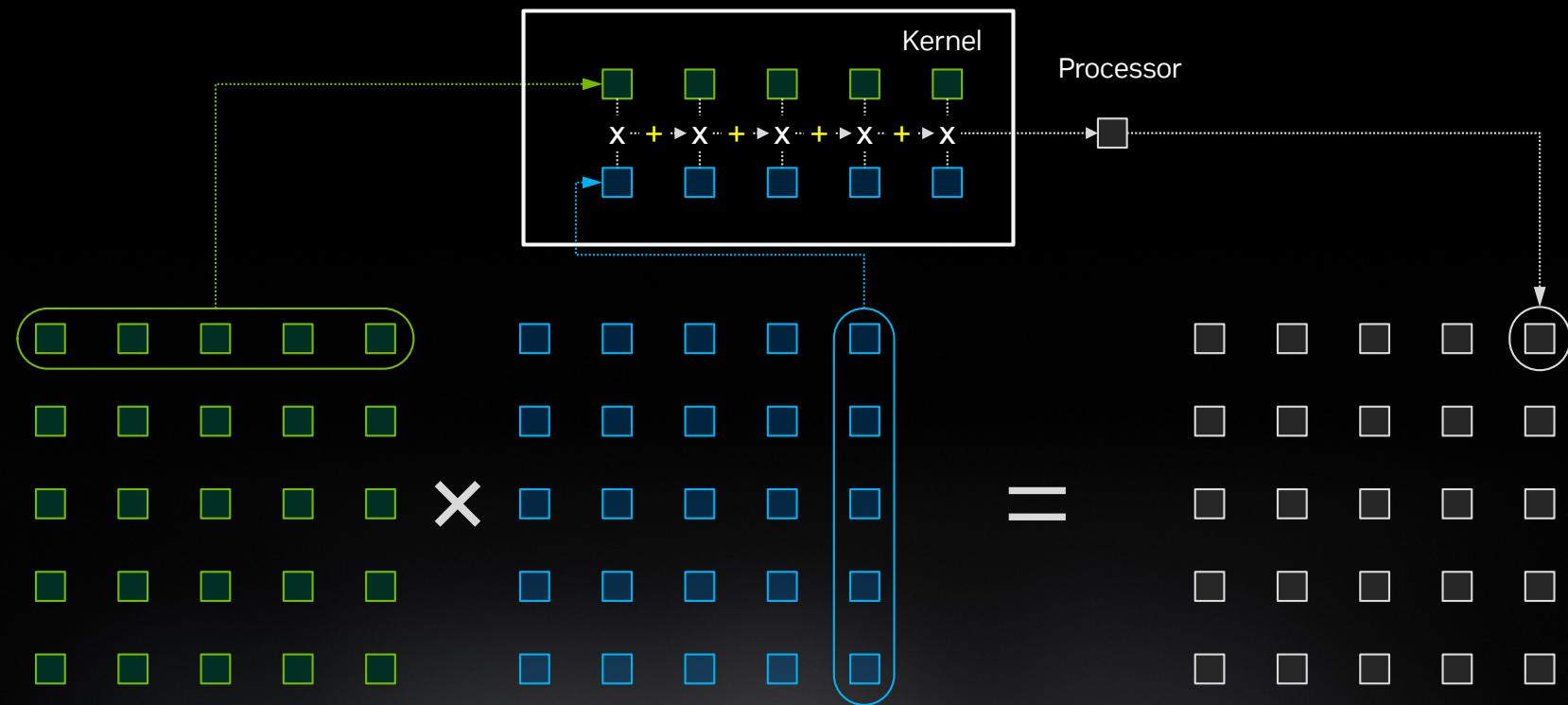
Matrix Multiplication

Can be carried out in parallel



Matrix Multiplication

Can be carried out in parallel



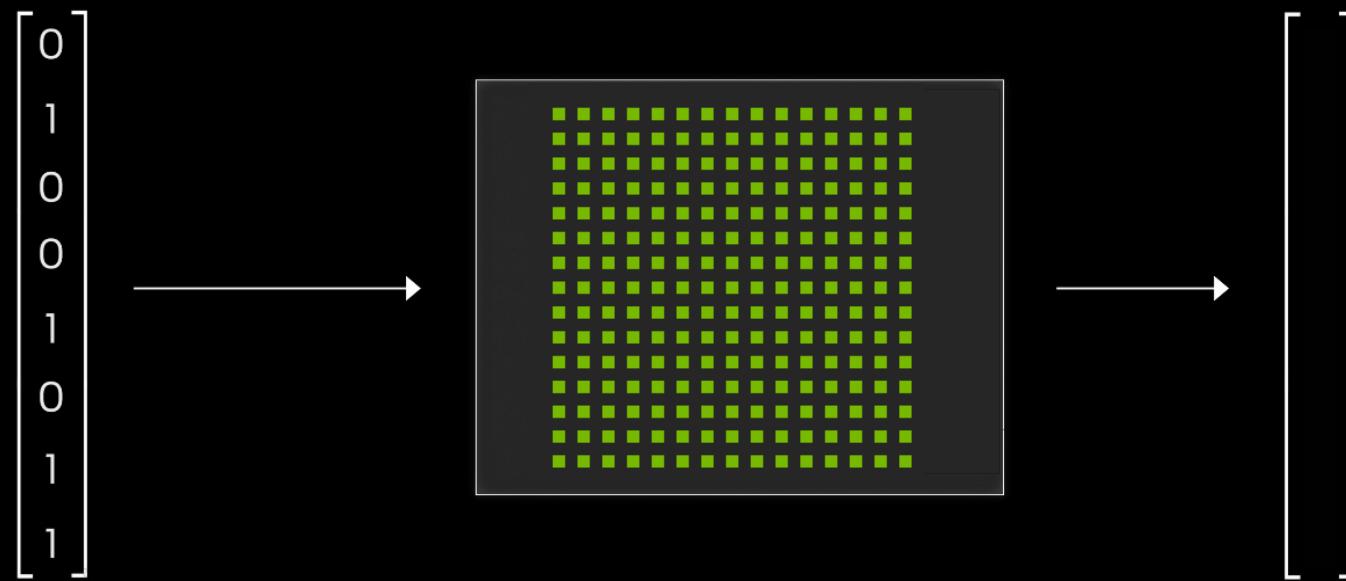
Synchronous



Asynchronous



Matrix Multiplication

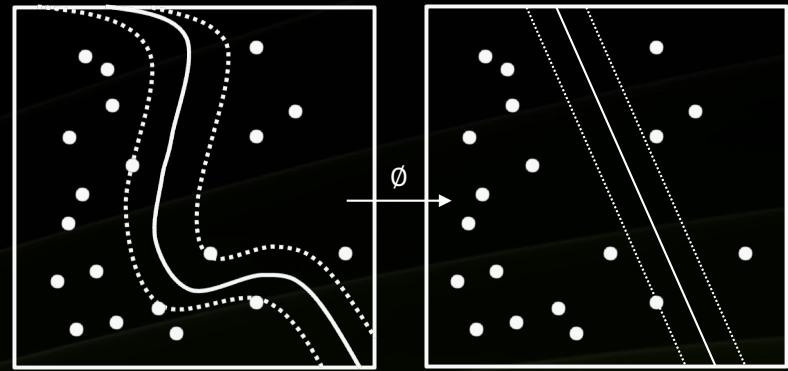


A quantum processor acting on N qubits
can be modeled by a $2^N \times 2^N$ matrix

Fraud Detection

HSBC Leverages CUDA-Q to Develop Improved Fraud Detection

- Fraudulent transactions: loss of \$1.9BN per year for UK alone
- Quantum-inspired methods may improve fraud detection
- Reduced false positives by 4%, improved true positives by 2%
- Run as 165 qubit classification problem on GPUs with CUDA-Q





Agenda

- Quantum circuits and quantum kernels – [CUDA-Q Lab 2](#)

- AI for Accelerated Quantum Supercomputing

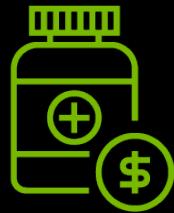
- Variational Algorithm and Adaptive Circuit Knitting

- Resources to learn more about Accelerated Quantum Supercomputing

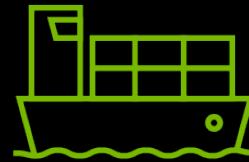
Quantum Computing's Broad Impact



EV chemistry



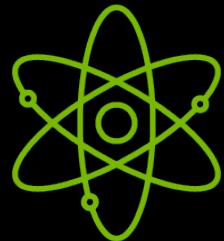
Drug discovery



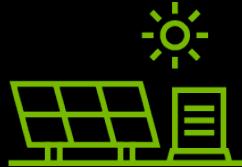
Logistics



Finance



Physics modelling



Materials

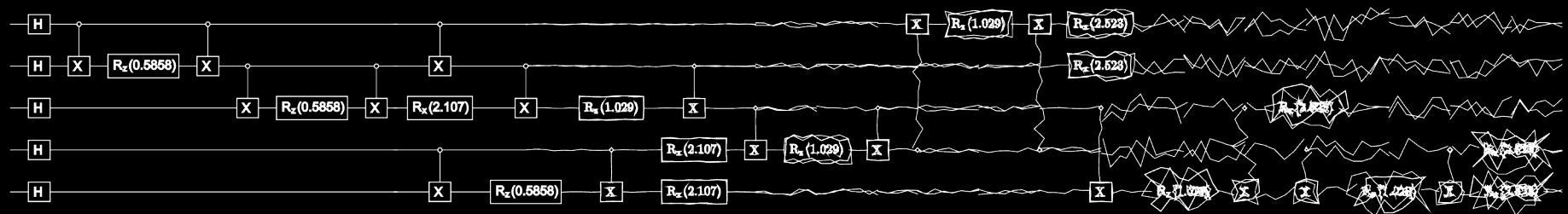


Nitrogen fixation



AI and ML

Noise Limits Today's Quantum Hardware

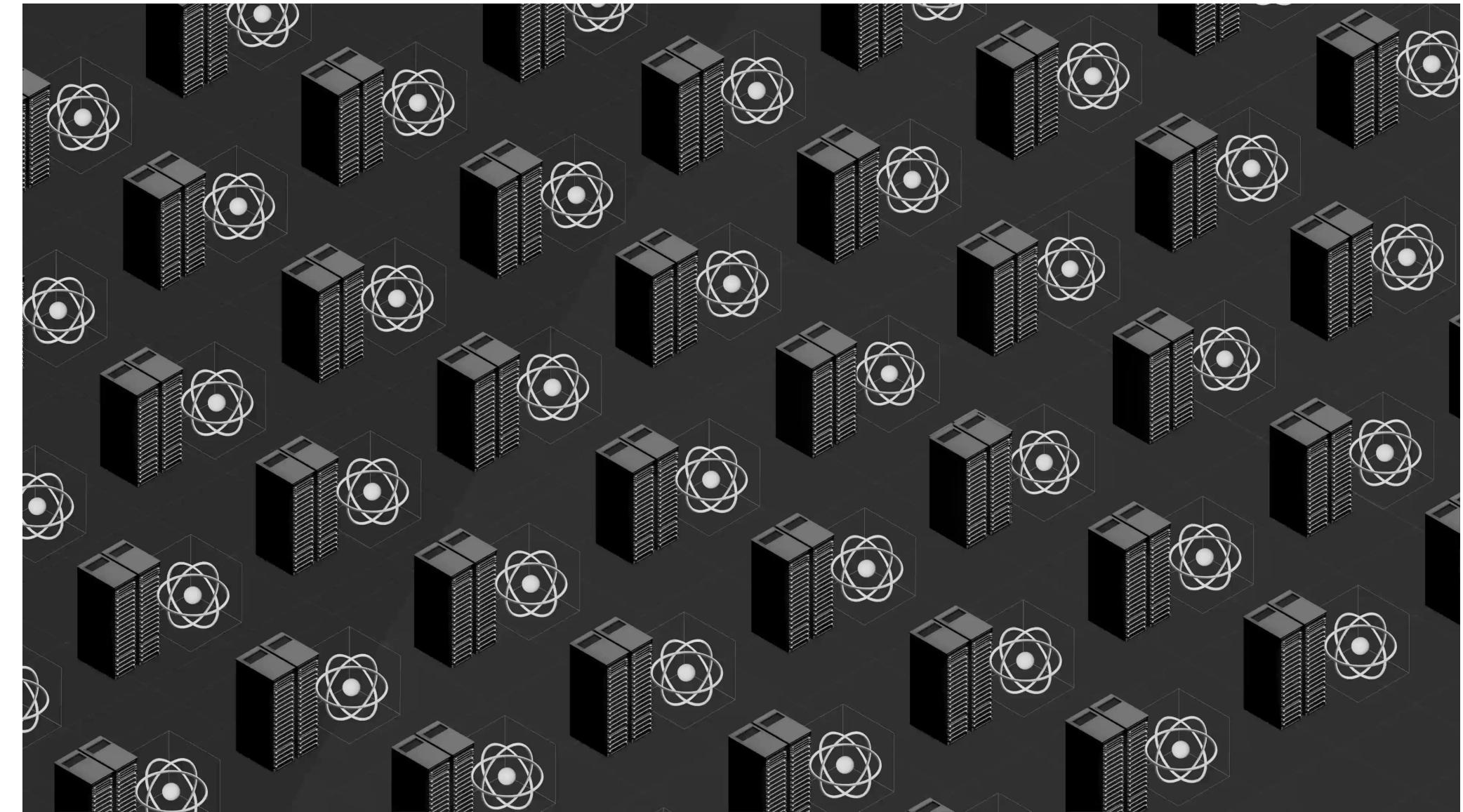


Noise limits computations on today's quantum hardware to just hundreds of operations



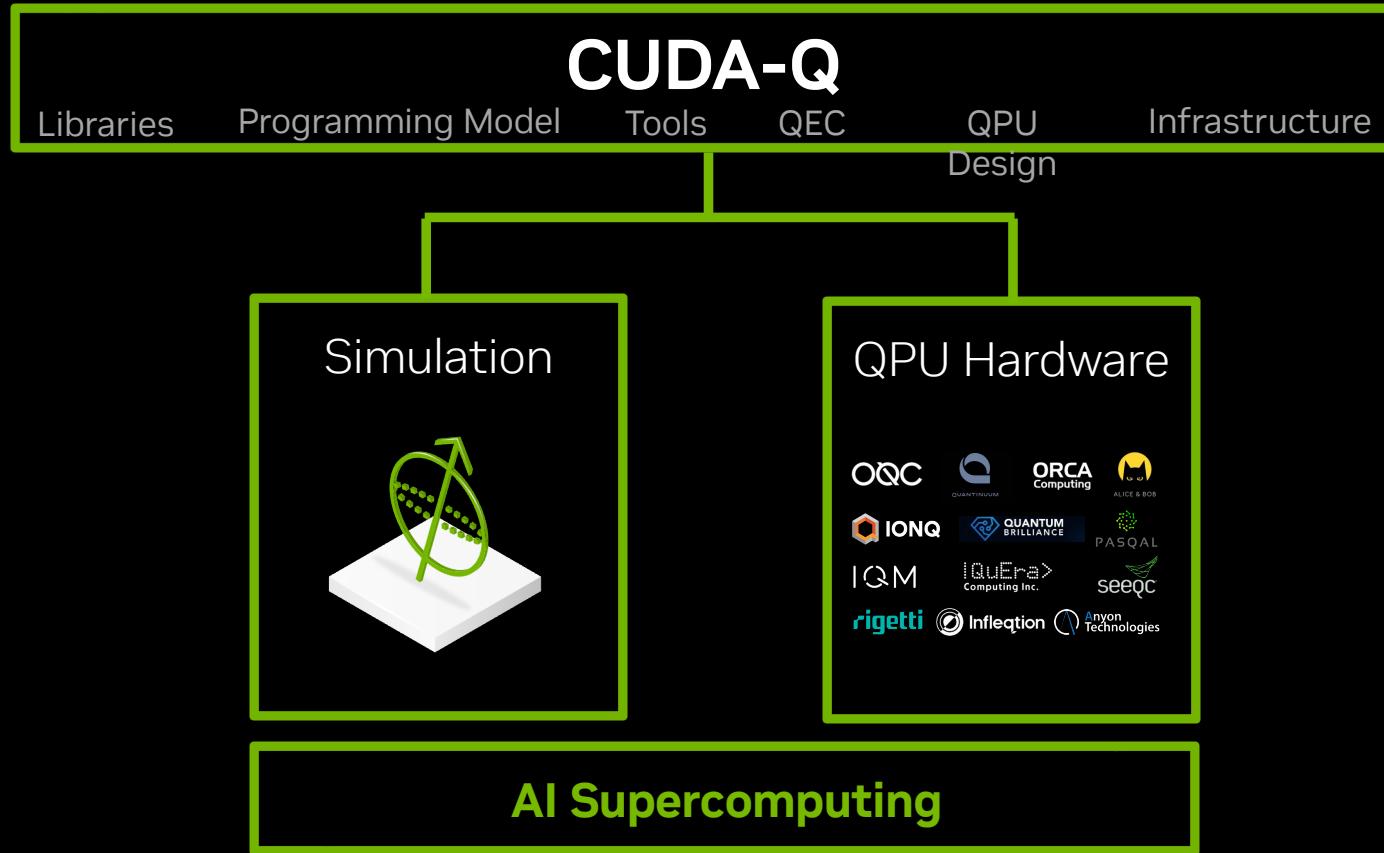
Agenda

- Quantum circuits and quantum kernels
- AI for Accelerated Quantum Supercomputing
- Variational Algorithm and Adaptive Circuit Knitting
- Resources to learn more about Accelerated Quantum Supercomputing

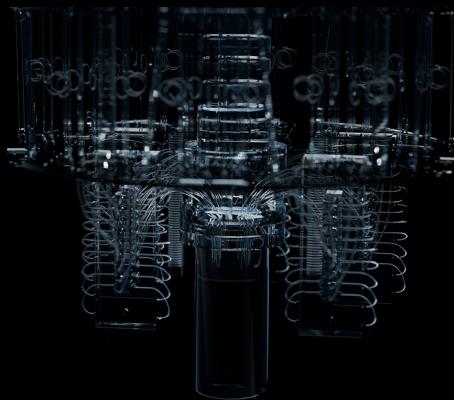


CUDA-Q

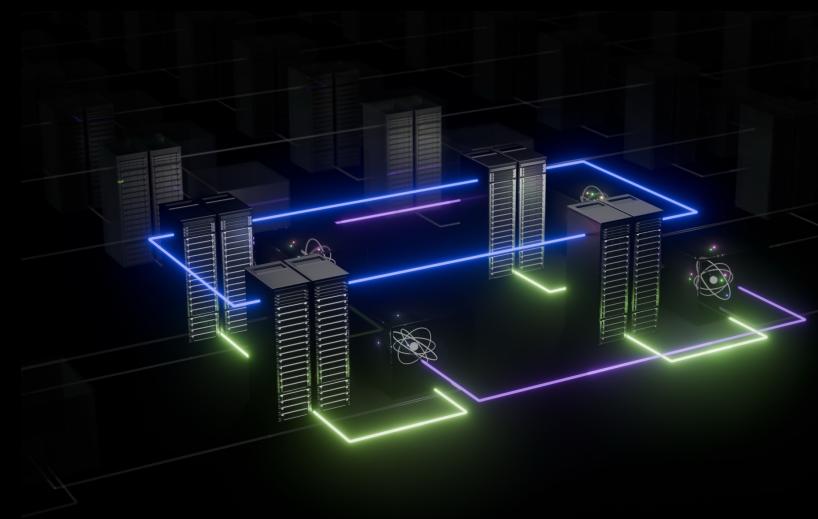
The platform for accelerated quantum computing



Accelerating the Journey From Qubits to Supercomputers

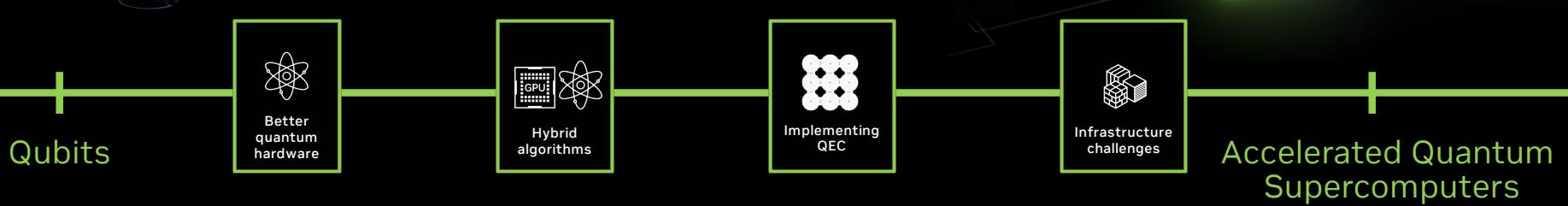
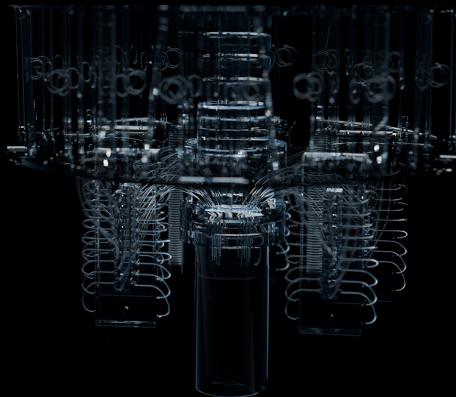


Qubits

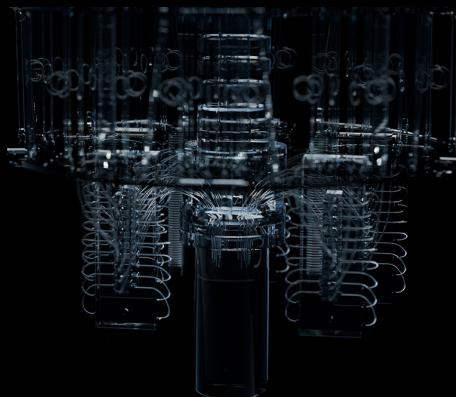


Accelerated Quantum
Supercomputers

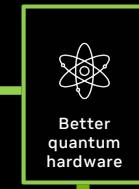
Accelerating the Journey From Qubits to Supercomputers



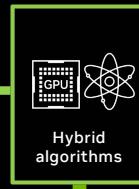
Accelerating the Journey From Qubits to Supercomputers



Qubits



Better
quantum
hardware



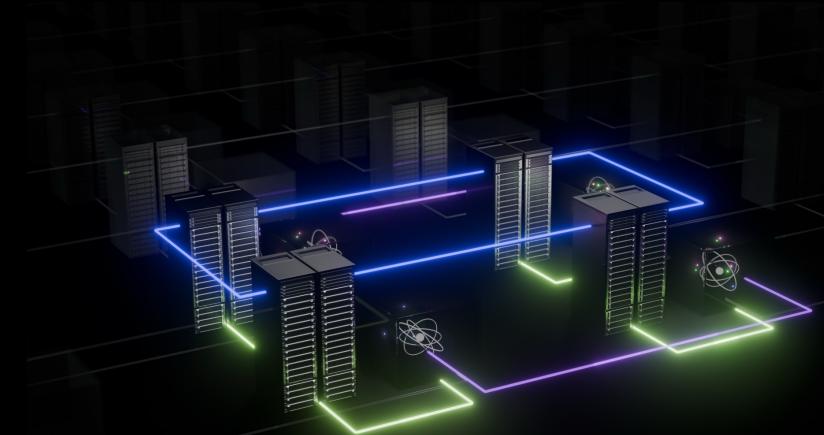
Hybrid
algorithms



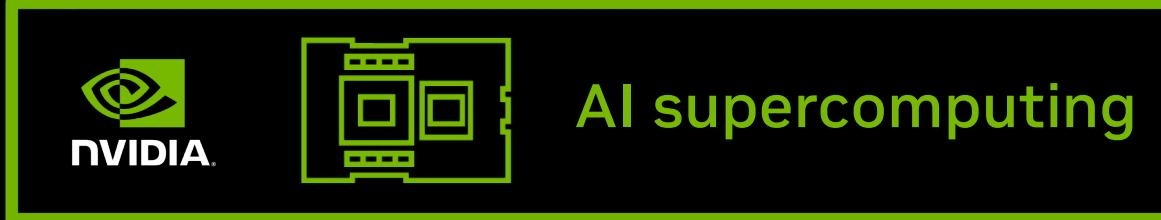
Implementing
QEC



Infrastructure
challenges

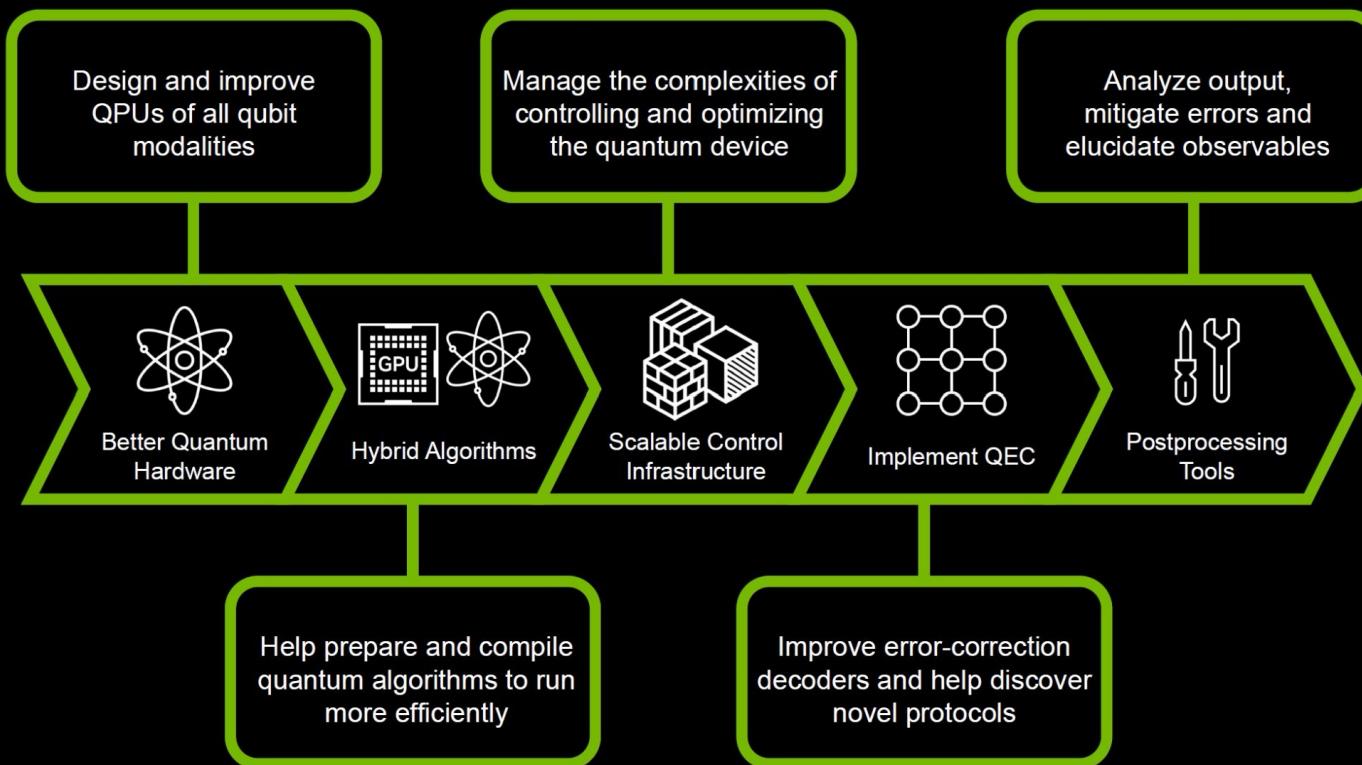


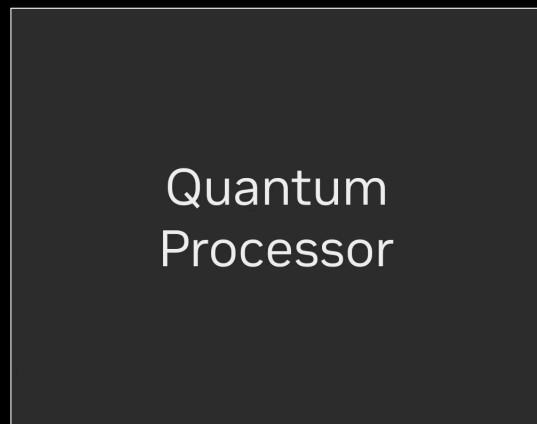
Accelerated Quantum
Supercomputers



Artificial Intelligence for Quantum Computing

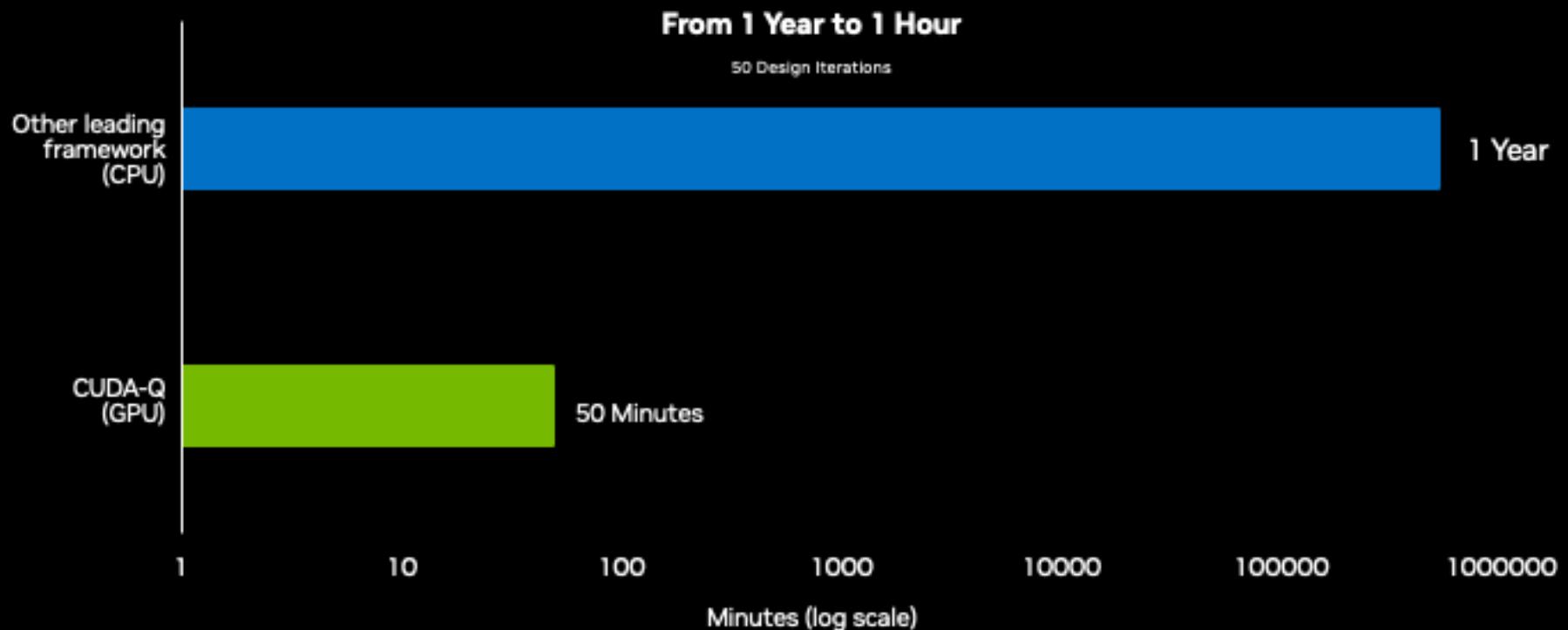
[arXiv:2411.09131](https://arxiv.org/abs/2411.09131)



$$\begin{bmatrix} 1 \\ 0 \\ 1 \\ 1 \\ 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}$$


Dynamics in CUDA-Q

Enabling QPU developers everywhere to accelerate their design process



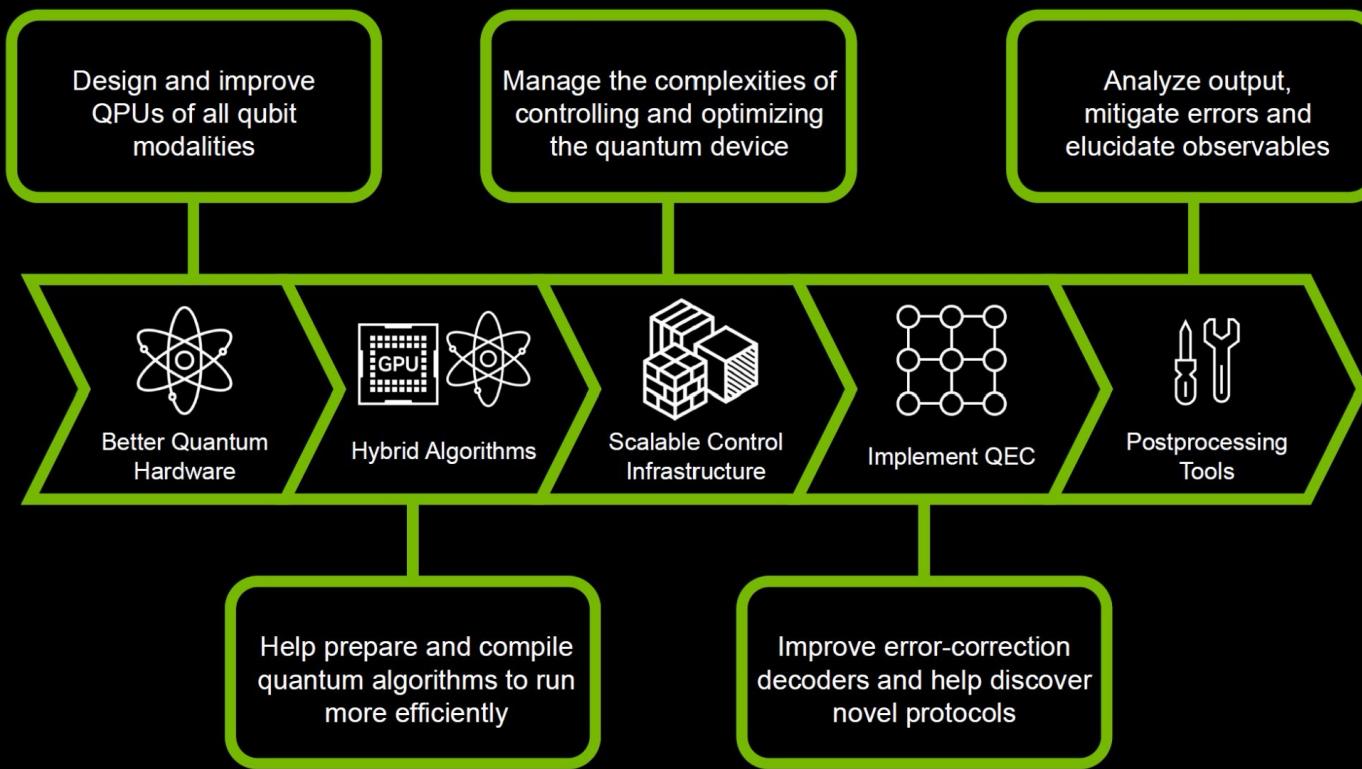
CPU: Intel Xeon 8480CL | GPU: DGX H100

Energy levels: 32 Transmon x 128 Resonator x 4 Purcell Filter



Artificial Intelligence for Quantum Computing

[arXiv:2411.09131](https://arxiv.org/abs/2411.09131)



AI for Error Correction

AI-driven code generation and decoding

AI for code generation

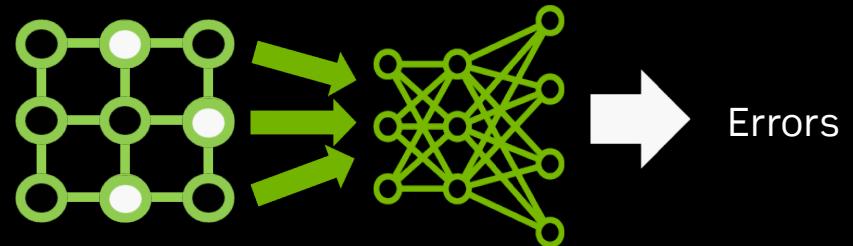
Error correcting code with specific properties are generated by reinforcement learning



Error correcting code

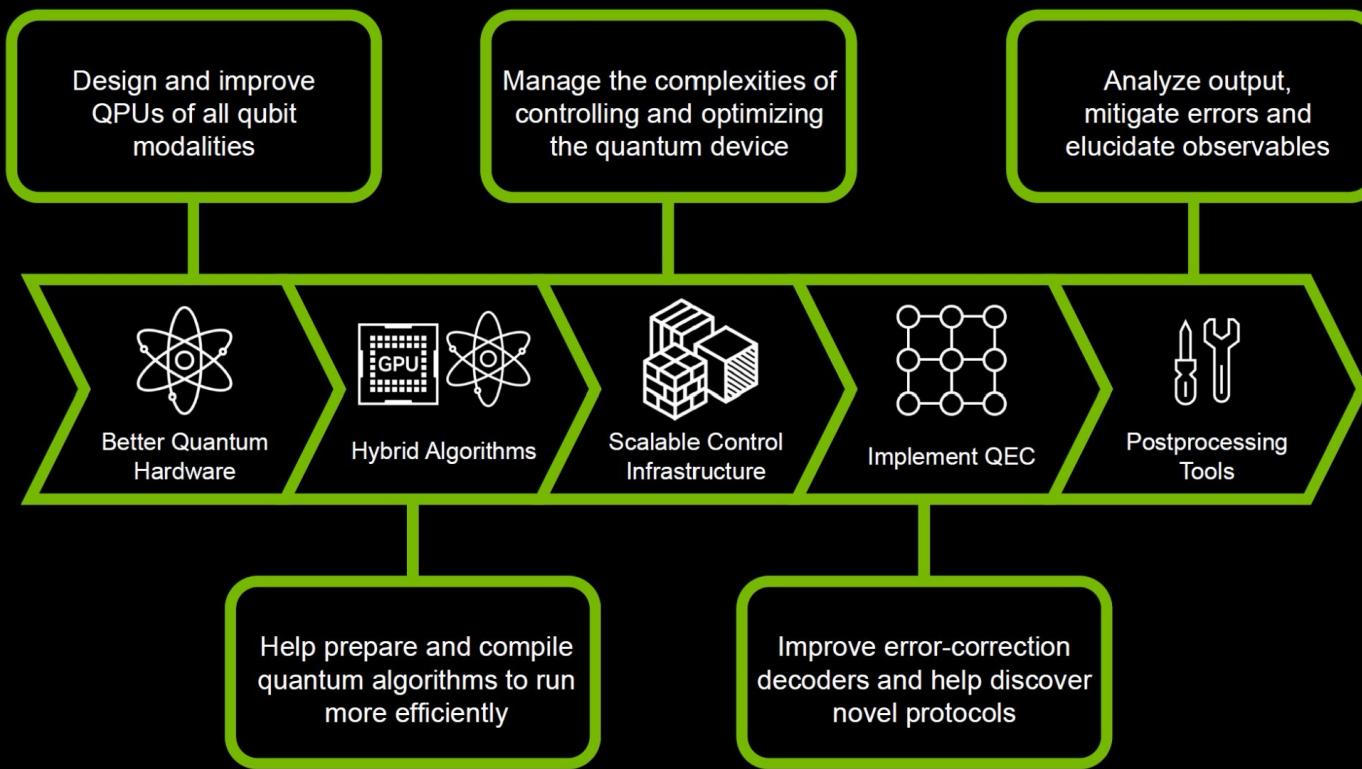
AI for decoders

The result of syndrome measurements are decoded by machine learning models



Artificial Intelligence for Quantum Computing

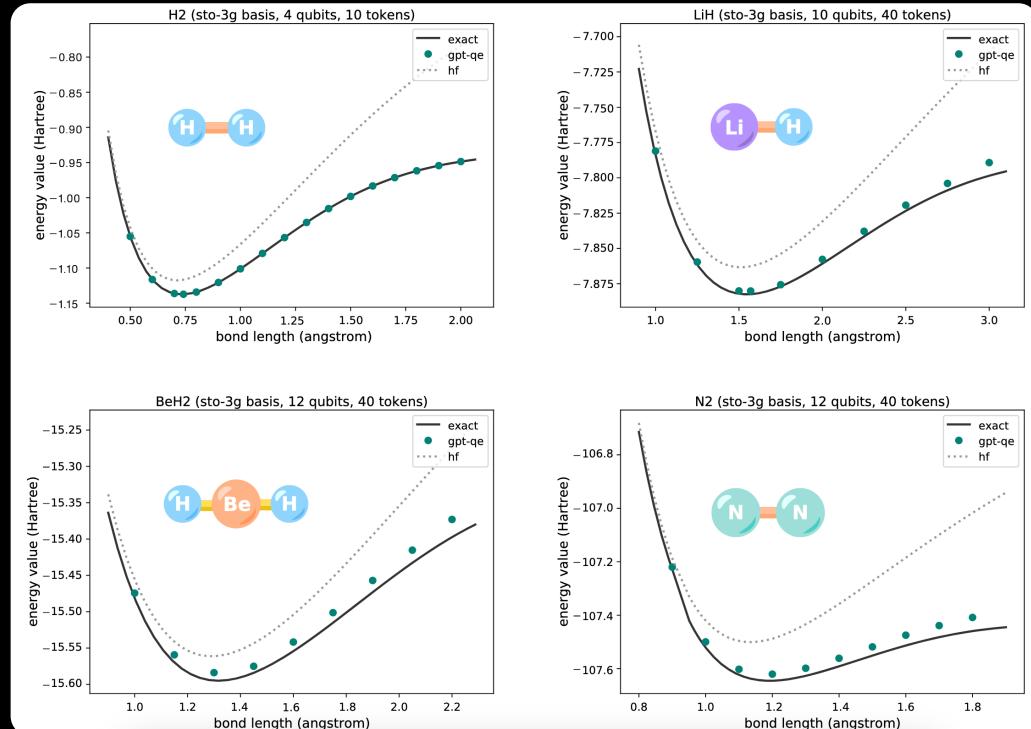
[arXiv:2411.09131](https://arxiv.org/abs/2411.09131)



Application to Ground State Search

GTP-QE used to generate circuits producing a molecular ground state

- Clear example of leveraging AI for QC
- Executed using CUDA-Q on A100 GPUs in Perlmutter supercomputer
- Can be extended to variety of novel Generative Quantum Algorithms (GQAs)
 - Potential extensions in drug discovery, materials science, and environmental applications.



The Generative Quantum Eigensolver

First demonstration of GPT-generated circuits in the literature

Goal: Find a circuit producing e.g. ground state

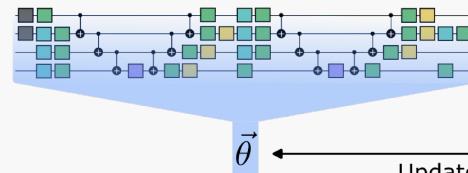
Optimization of some possible space of circuits for desired output

VQE

Optimization parameters are part of quantum circuit

- Leads to issues with local minima and barren plateaus

Ansatz Circuit



QPU



$$\frac{\partial E}{\partial \theta}$$

Update $\delta\theta$

VQE



UNIVERSITY OF
TORONTO



<https://arxiv.org/pdf/2401.09253.pdf>

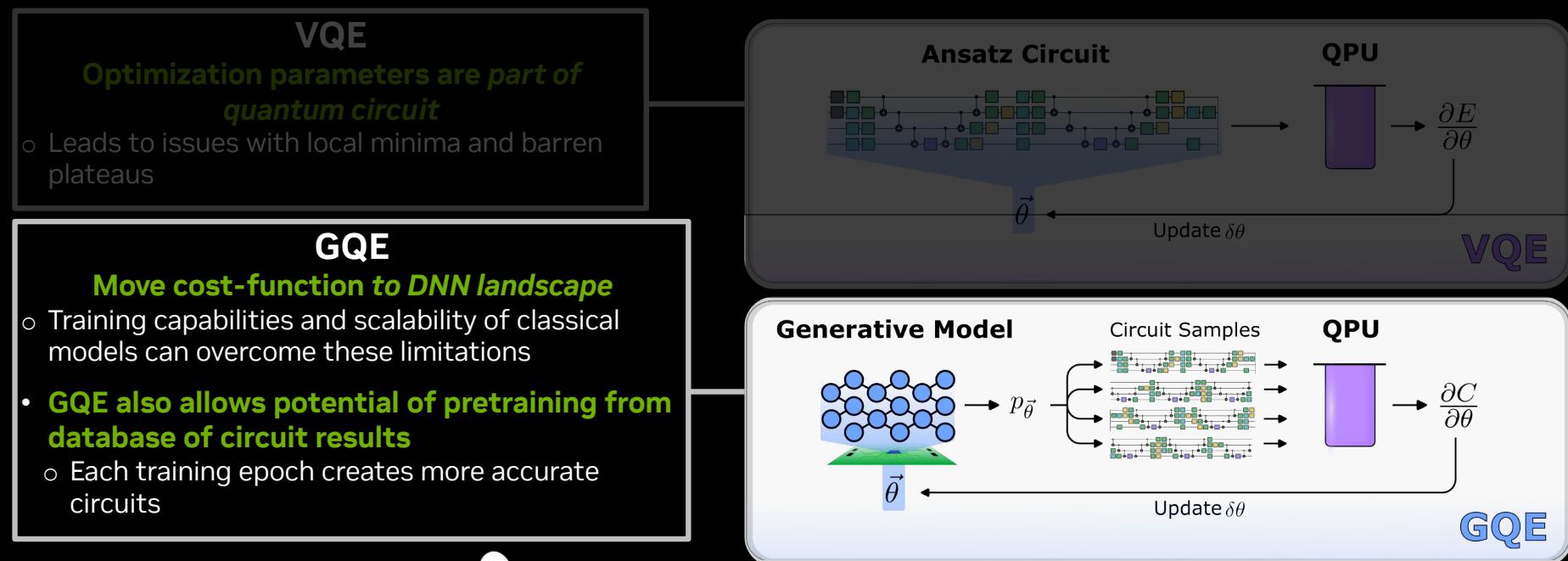


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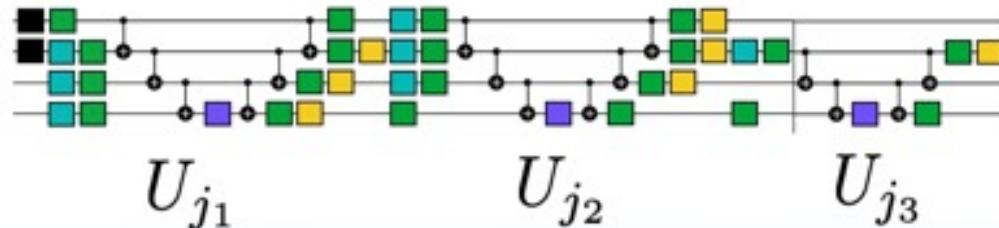


AI Assisted circuit design

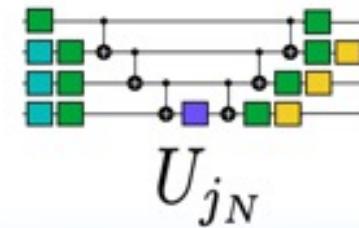
$\vec{j} \sim$ "Once upon a time . . . happily ever after"
word_{j₁} word_{j₂} word_{j₃} word_{j₄} . . . word_{j_{N-2}} word_{j_{N-1}} word_{j_N}

LLM

$\vec{j} \sim$



...



GPT-QE

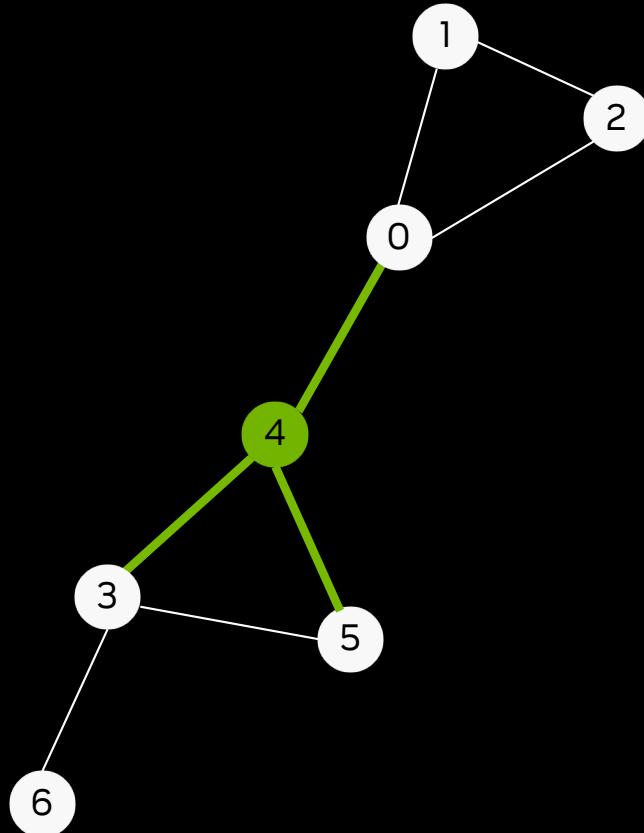


Agenda

- Quantum circuits and quantum kernels
- AI for Accelerated Quantum Supercomputing
- Variational Algorithm Adaptive Circuit Knitting Example – QAOA Lab 1
- Resources to learn more

Max Cut Problem

Identify a 2-coloring of the vertices to
maximize the number of edges between vertices of different colors



What's the
max cut of
this graph?

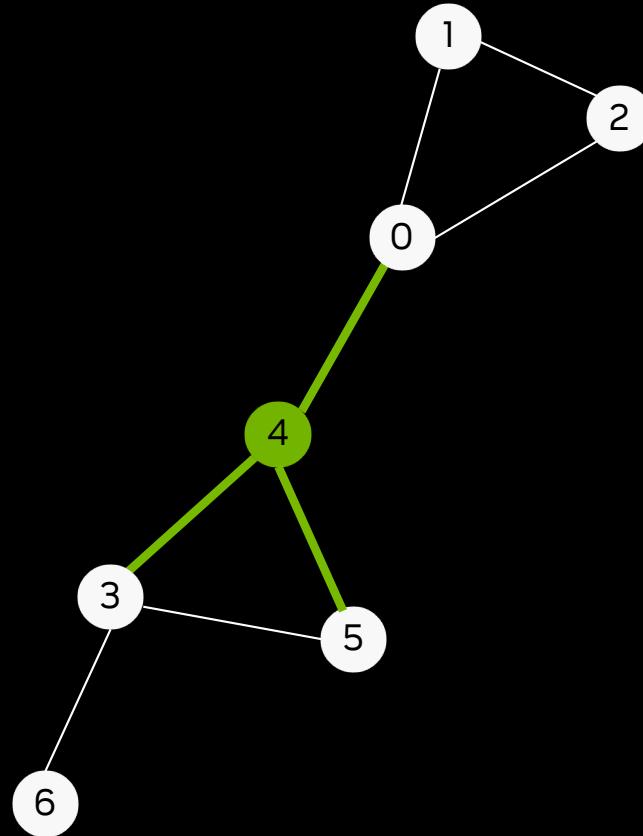


0
0
0
0
1
0
0

Max Cut Problem

Identify a 2-coloring of the vertices to
maximize the number of edges between vertices of different colors

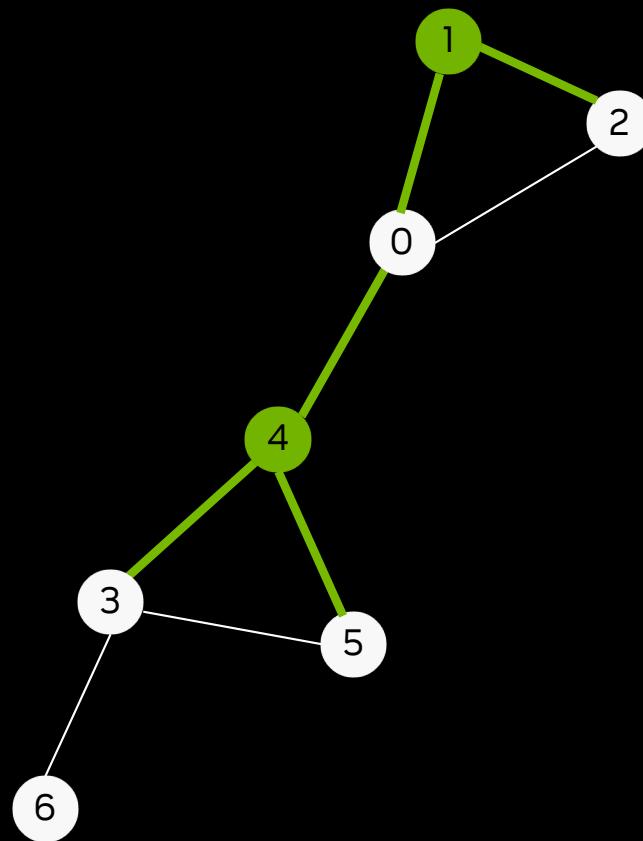
0
0
0
0
1
0
0



Max Cut Problem

Identify a 2-coloring of the vertices to
maximize the number of edges between vertices of different colors

0
1
0
0
1
0
0



Max Cut Problem

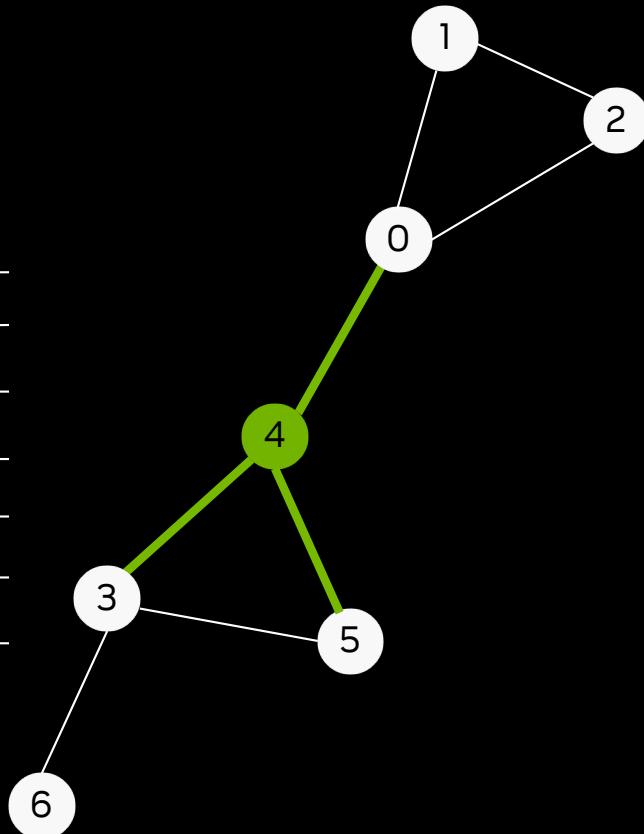
Identify a 2-coloring of the vertices to
maximize the number of edges between vertices of different colors

0
0
0
0
1
0
0

q_0
 q_1
 q_2
 q_3
 q_4
 q_5
 q_6

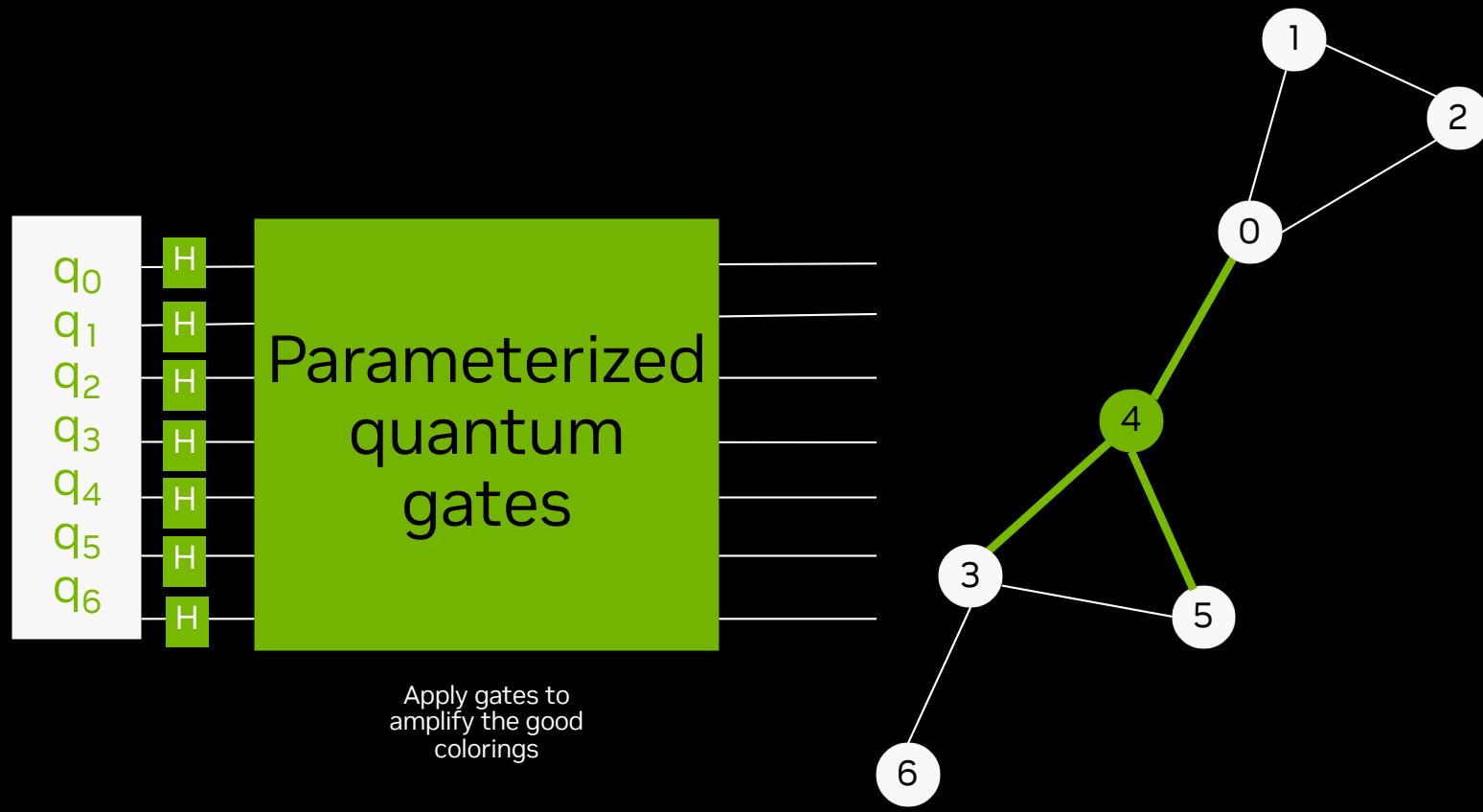
One
coloring

Superposition of
all colorings



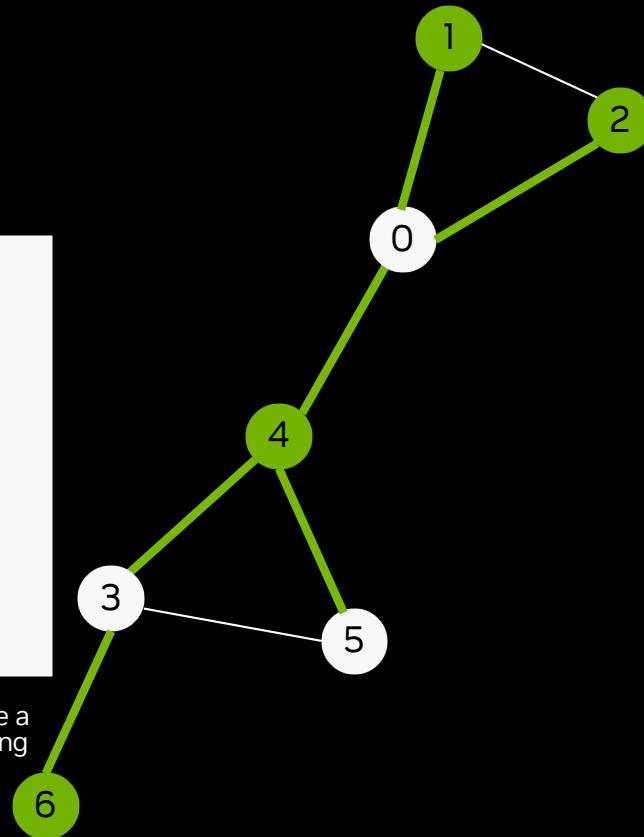
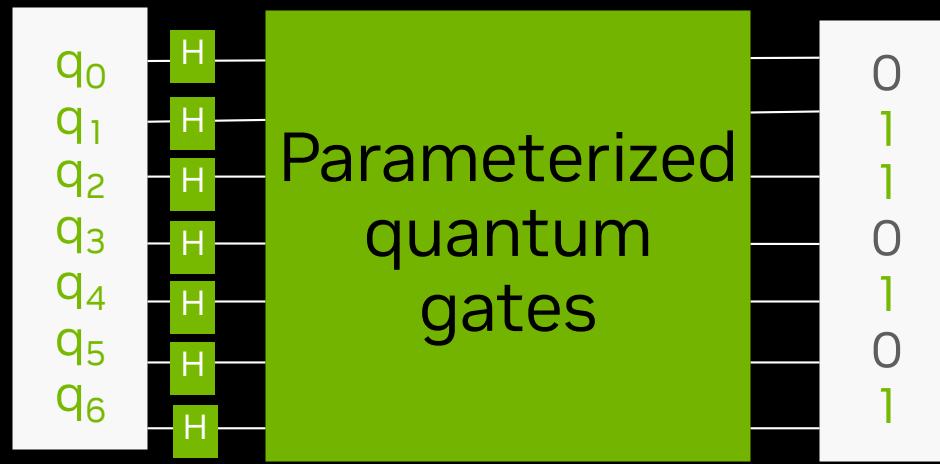
Max Cut Problem

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Max Cut Problem

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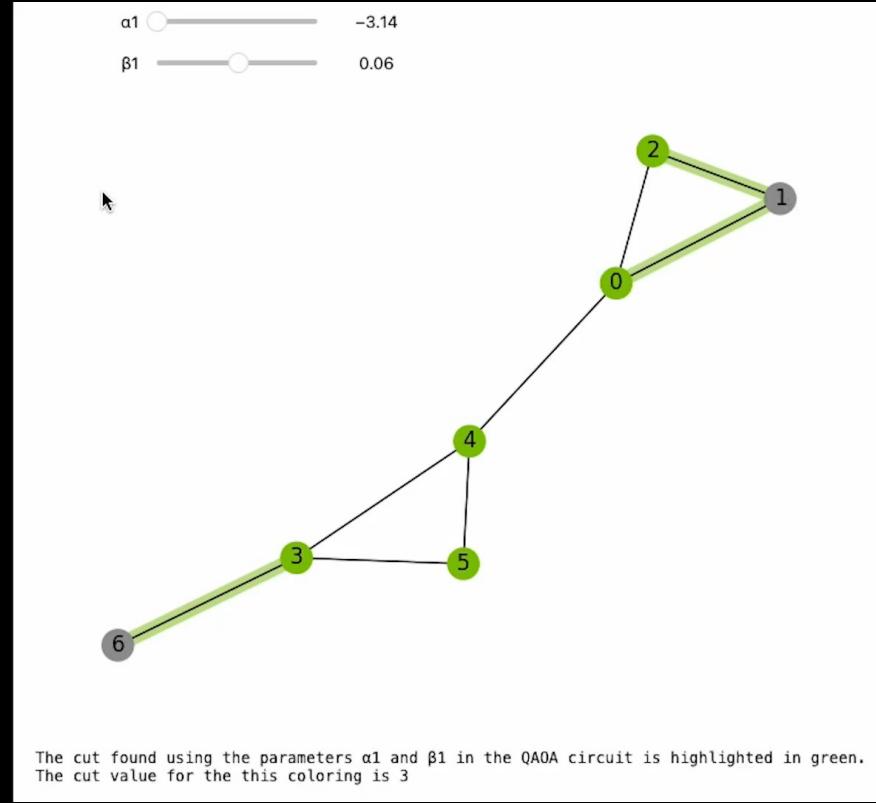


Learning the parameter values

Identify a 2-coloring of the vertices to
maximize the number of edges between vertices of different colors

Quantum
computation
with parameters
 α_1 and β_1

0
1
0
0
0
0
1



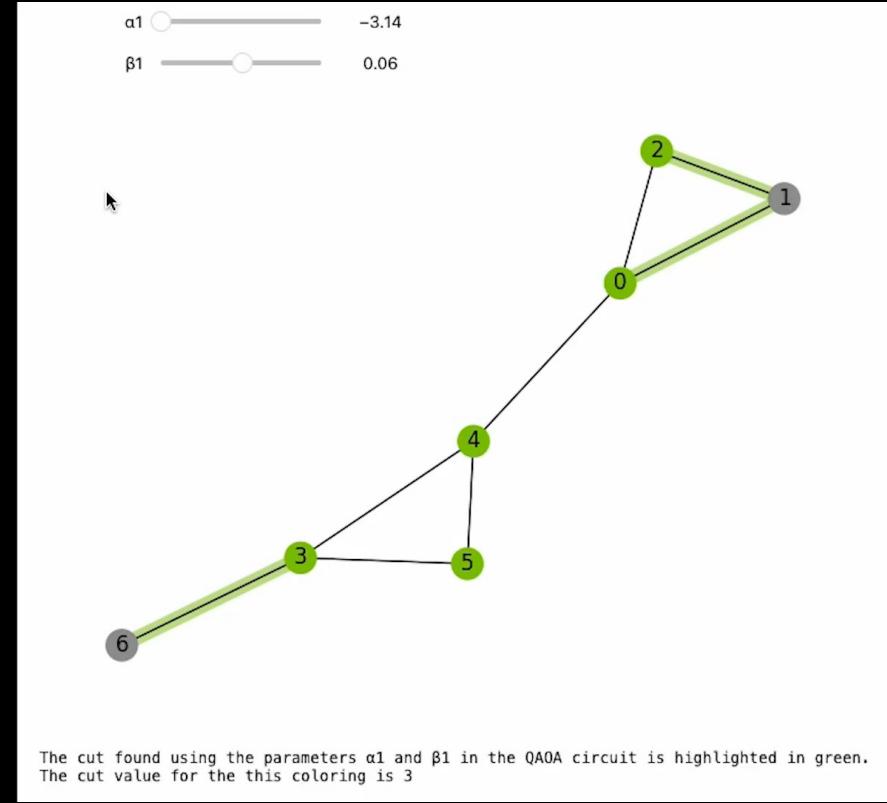
Learning the parameter values

Identify a 2-coloring of the vertices to
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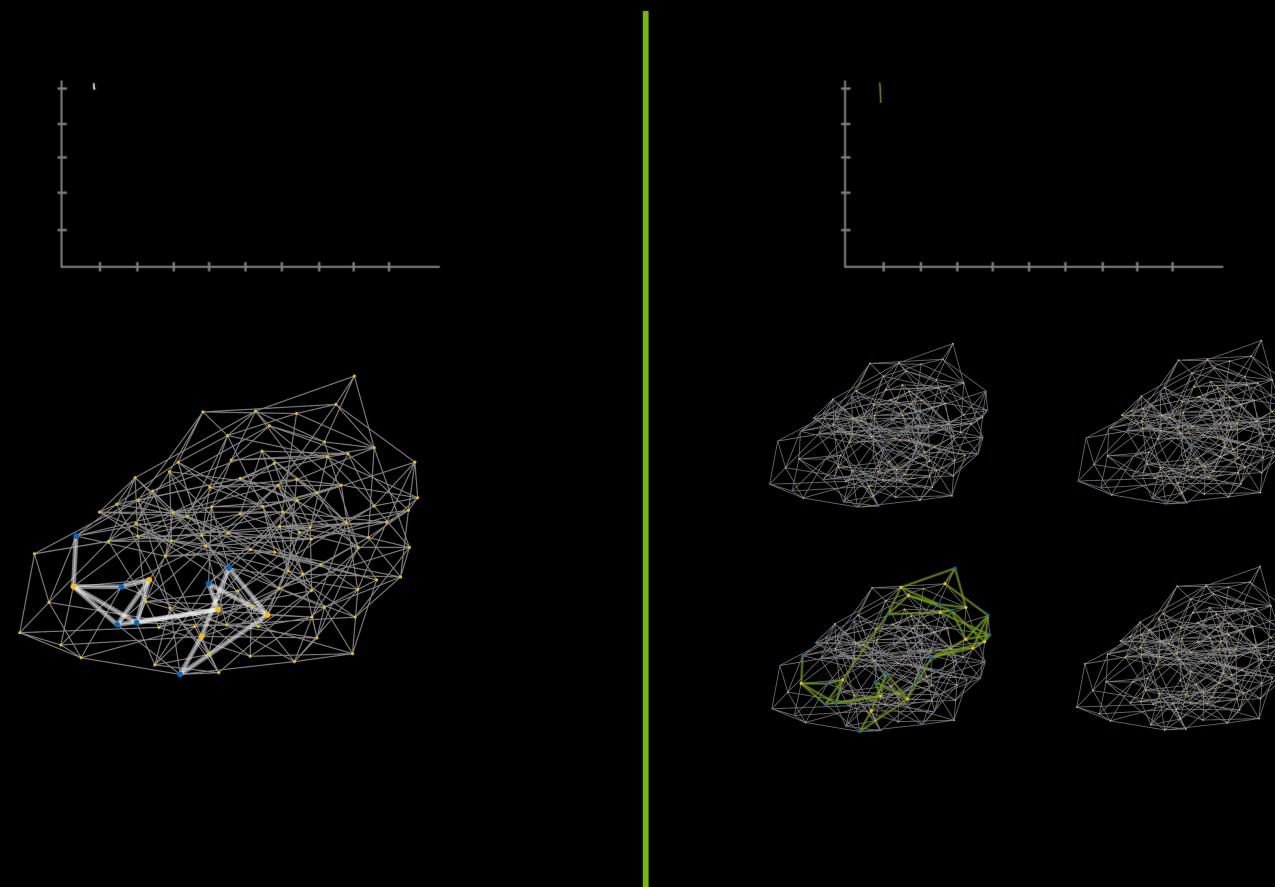
Quantum
computation
with parameters
 α_1 and β_1

Classical
optimizer to
update
parameter values

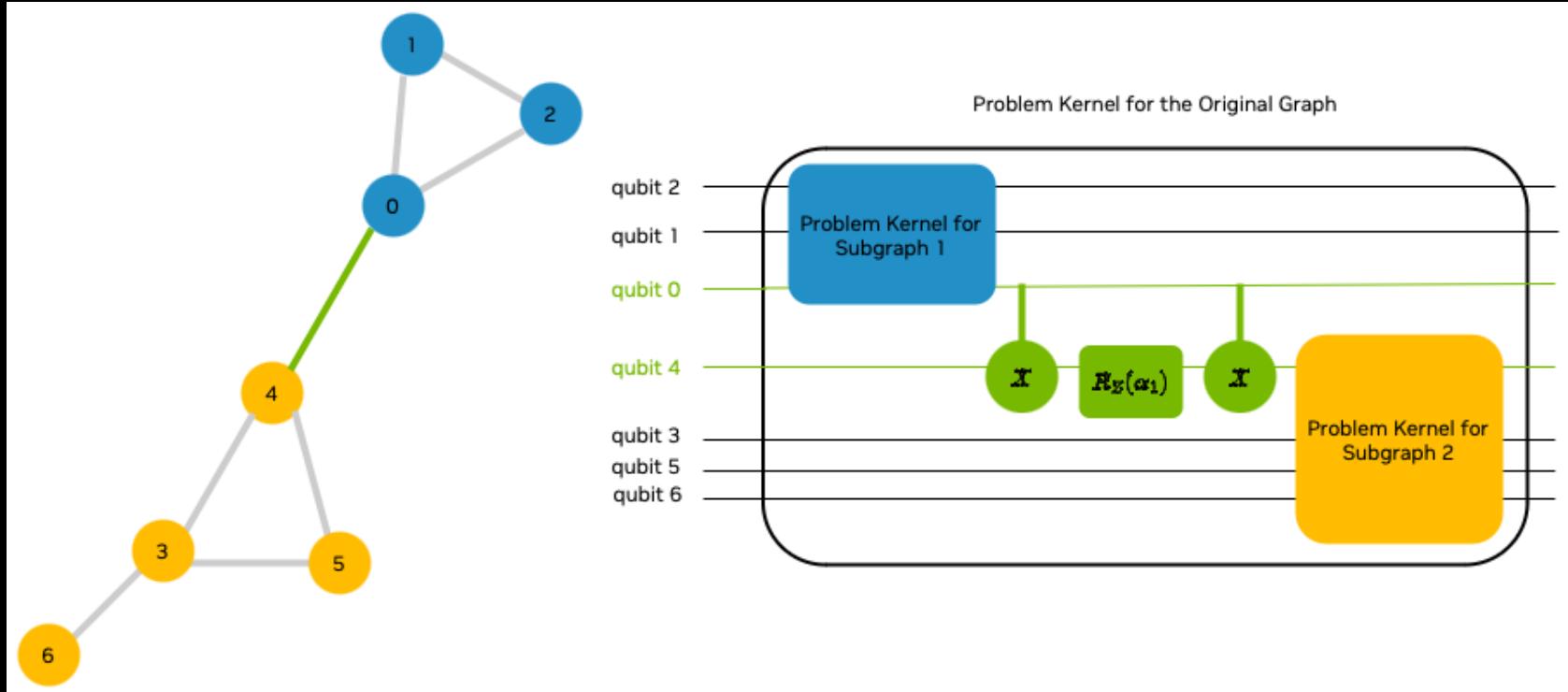
0
1
0
0
0
0
1



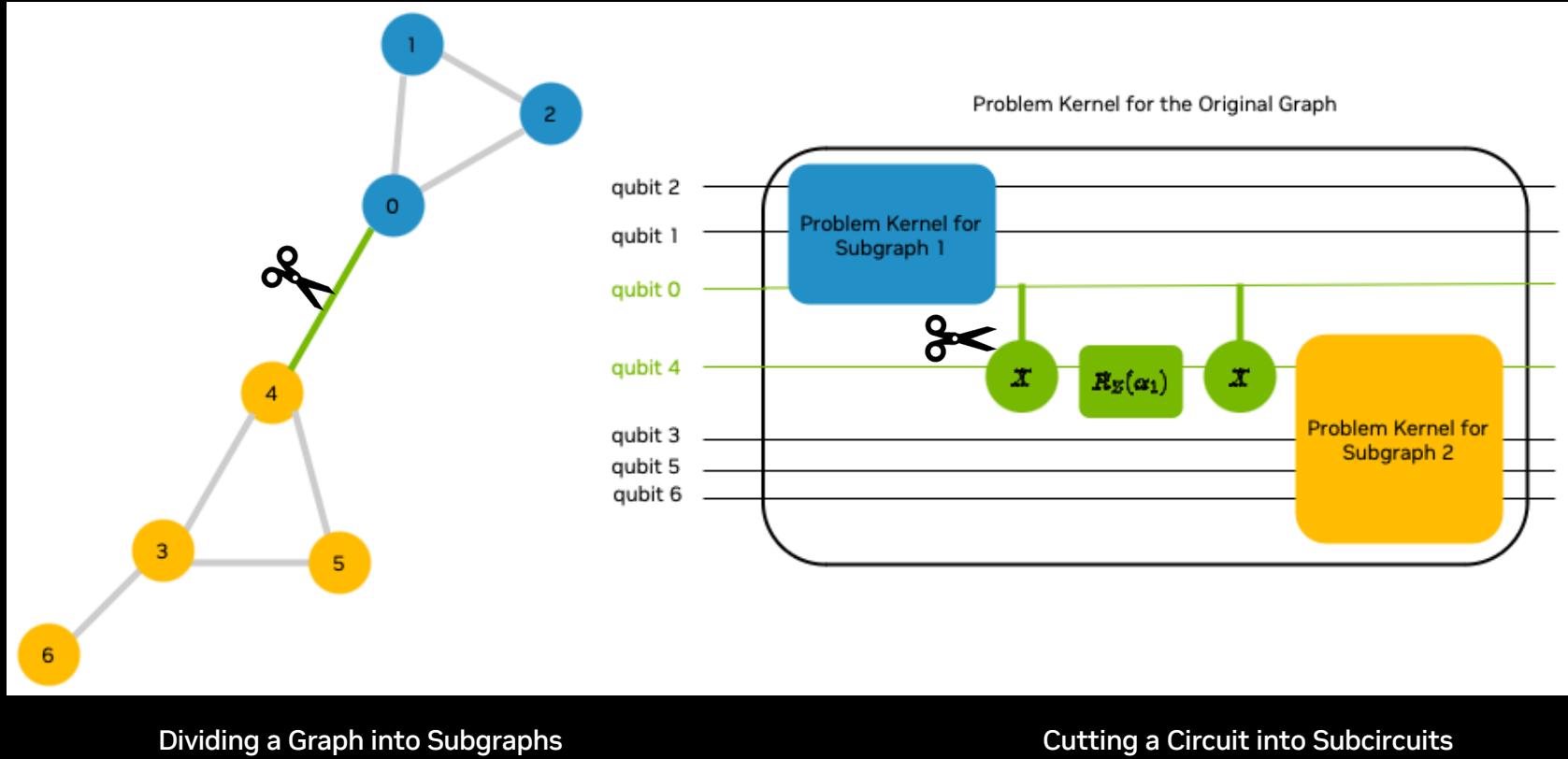
Max Cut Example to Illustrate Circuit Cutting



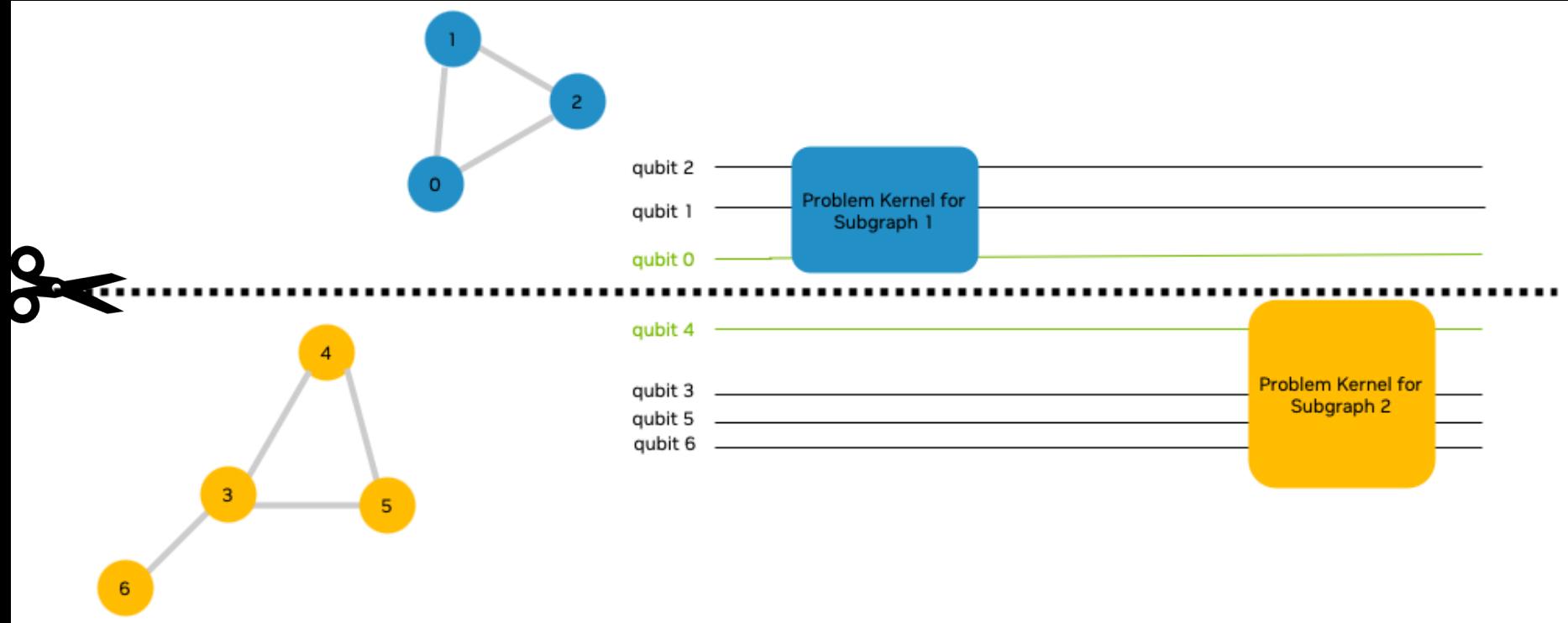
Visualizing Circuit Cutting



Visualizing Circuit Cutting



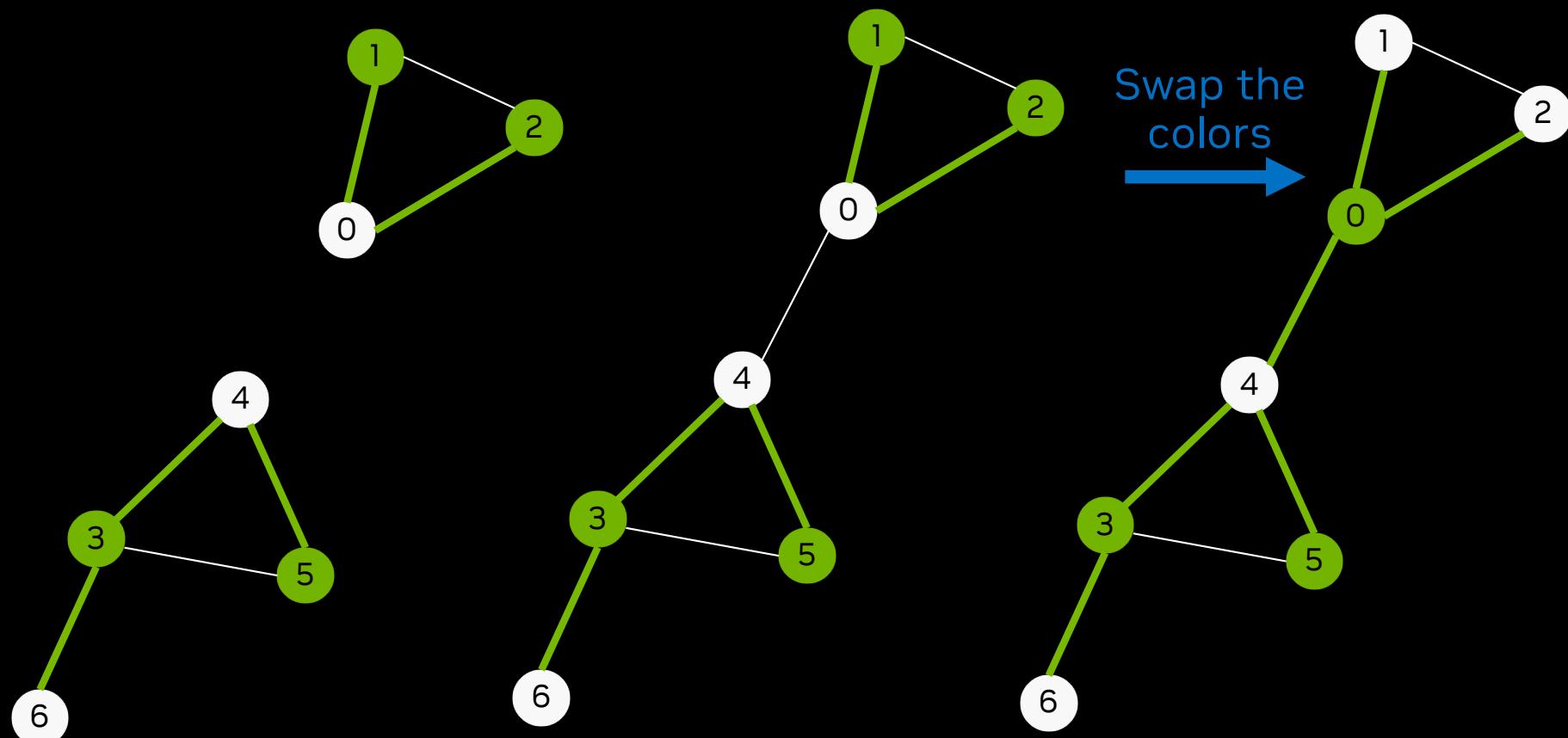
Visualizing Circuit Cutting



Dividing a Graph into Subgraphs

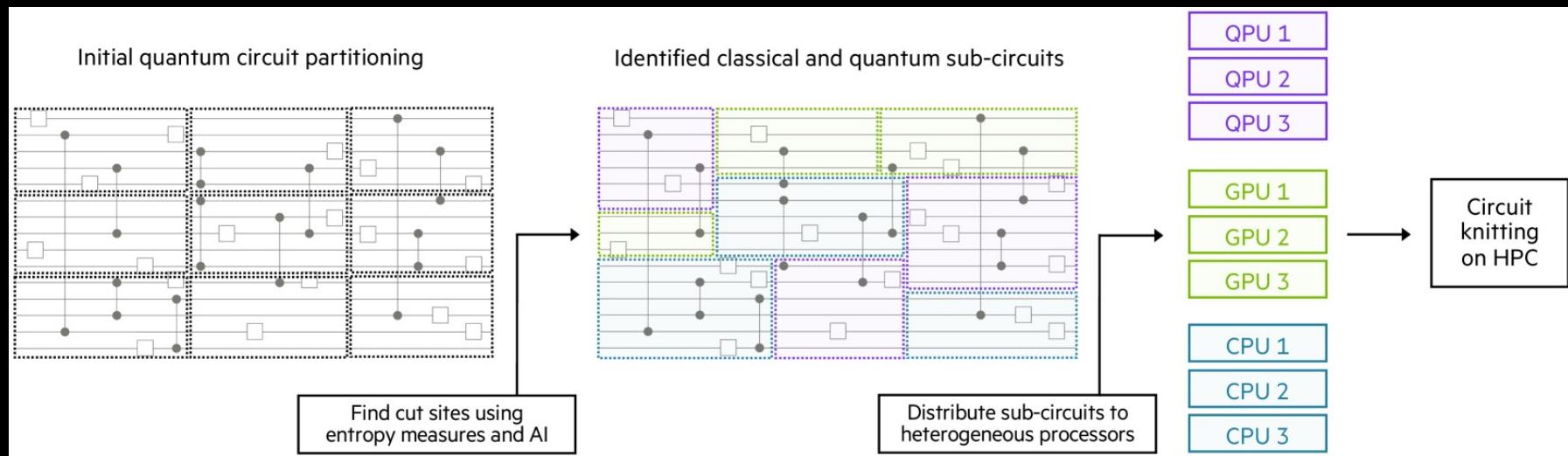
Cutting a Circuit into Subcircuits

Visualizing Circuit Knitting



Distributed Quantum Computing with Adaptive Circuit Knitting

To overcome the exponential overhead of traditional circuit knitting



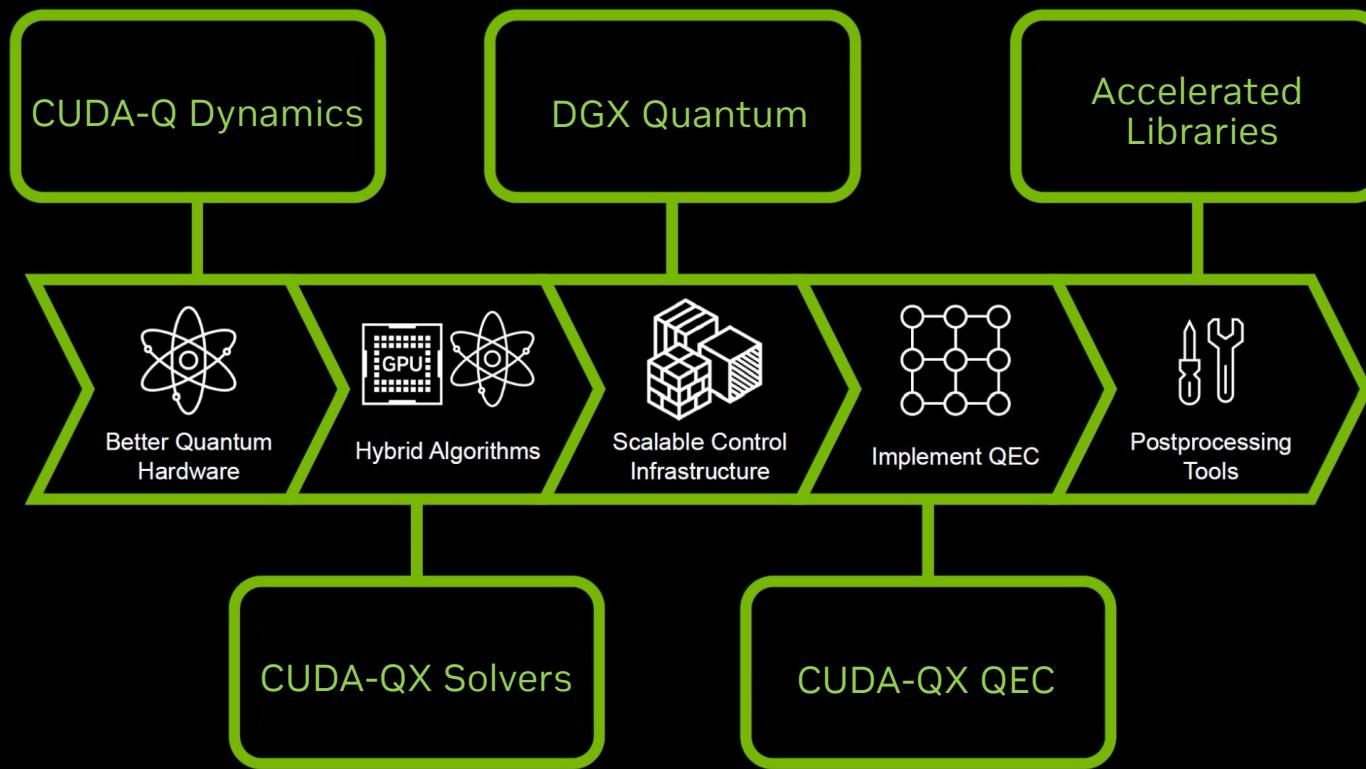
<https://arxiv.org/abs/2411.10406>



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Artificial Intelligence for Quantum Computing



Quantum: Not Just for Physicists

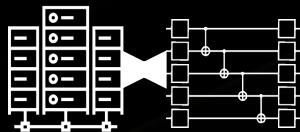
Overcoming these challenges requires broad spectrum of expertise



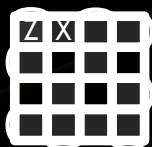
Qubit Fidelity
99.99% 2-Qubit Gate Fidelity



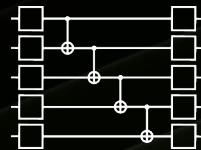
Qubit Scale
100k-1M+ Qubits for FTQC



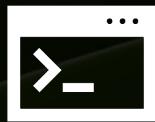
HPC Integration
Sub-Microsecond HPC-QC Latency



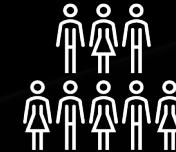
Error Correction
Methods that Scale to Large Quantum Systems



Algorithms
Algorithms with Exponential Speed-up



Developer Tools
Integrate with Scientific Computing
Familiar to non-Quantum Physicists



Physicists



Engineers



Computer Scientists



Developers



Mathematicians



Chemists



Biologists



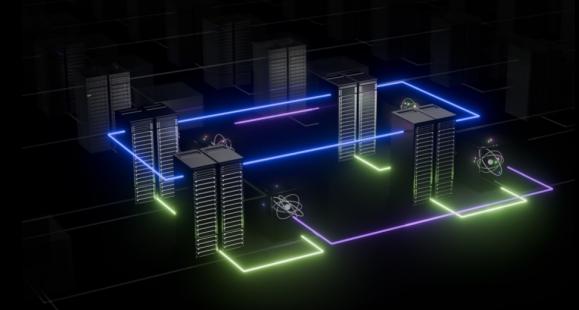
Subject Matter Experts



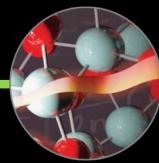
Students

CUDA-Q Academic

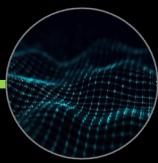
<https://github.com/NVIDIA/cuda-q-academic>



Today's Systems



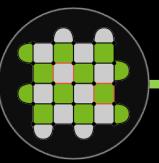
Quantum Algorithm
and Hybrid Application
Development



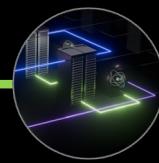
Qubit Design
EDA



GPU Simulations to
Generate
Quantum Data



Quantum Error
Correction



Quantum Computing
Deployments

CUDA-Q
Academic
Modules

Quantum
Applications to
Finance

Dynamics 101

Quick Start to
Quantum
Computing

QEC 101

Divide and
Conquer for
Max Cut

Find out more

NVIDIA Quantum

<https://www.nvidia.com/en-us/solutions/quantum-computing/>

CUDA-Q v0.10 Now Available

Python – Install from PyPi

C++ – <https://github.com/NVIDIA/cuda-quantum/releases>

CUDA-Q Academic

Educational resources for CUDA-Q

(<https://github.com/NVIDIA/cuda-q-academic>)



