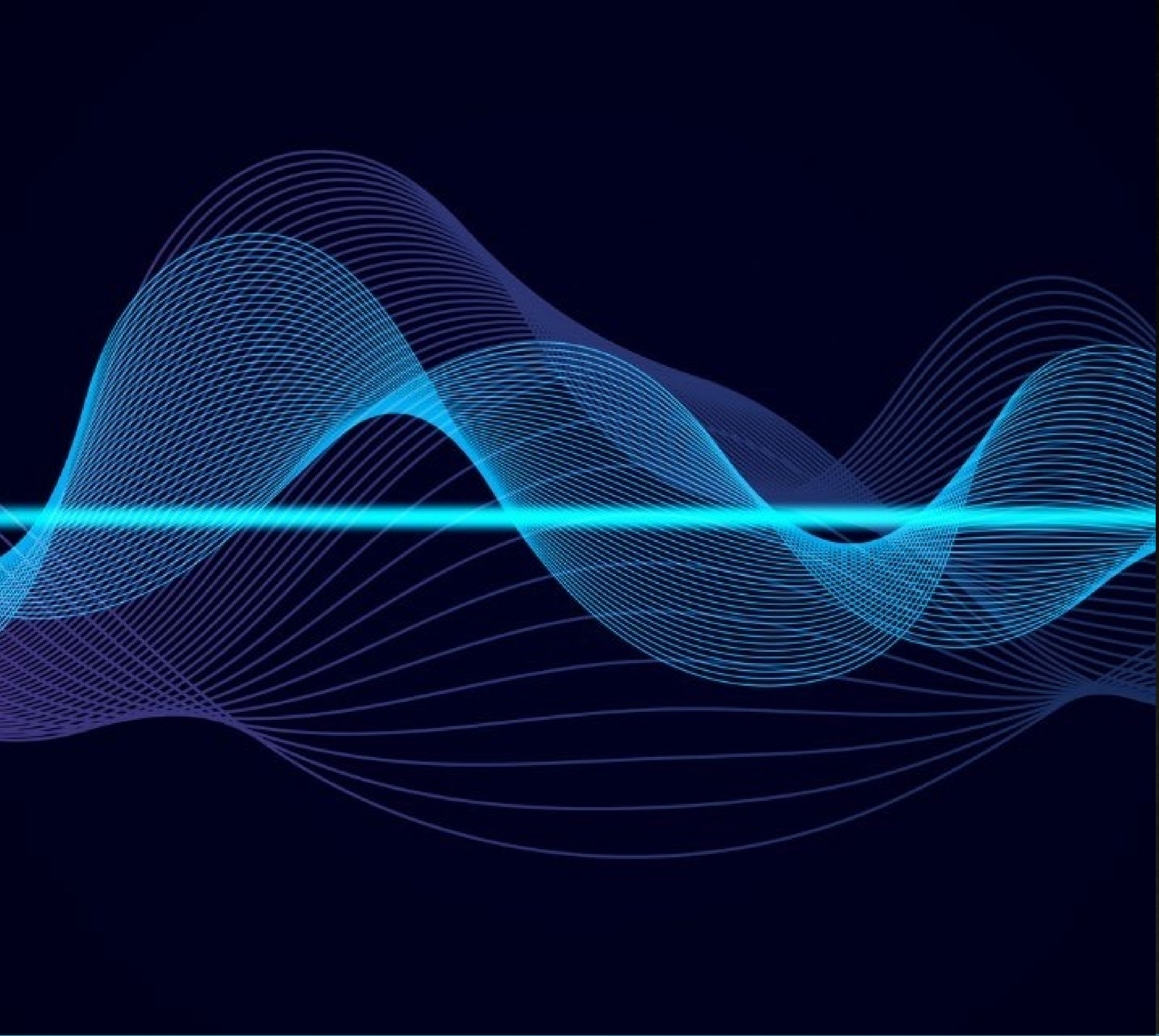


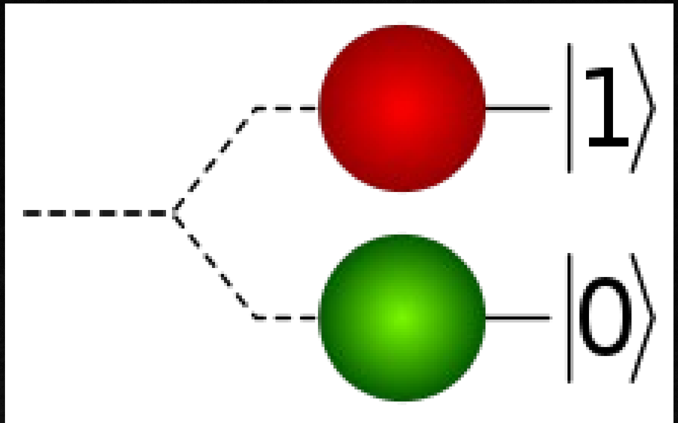
Computational Physics

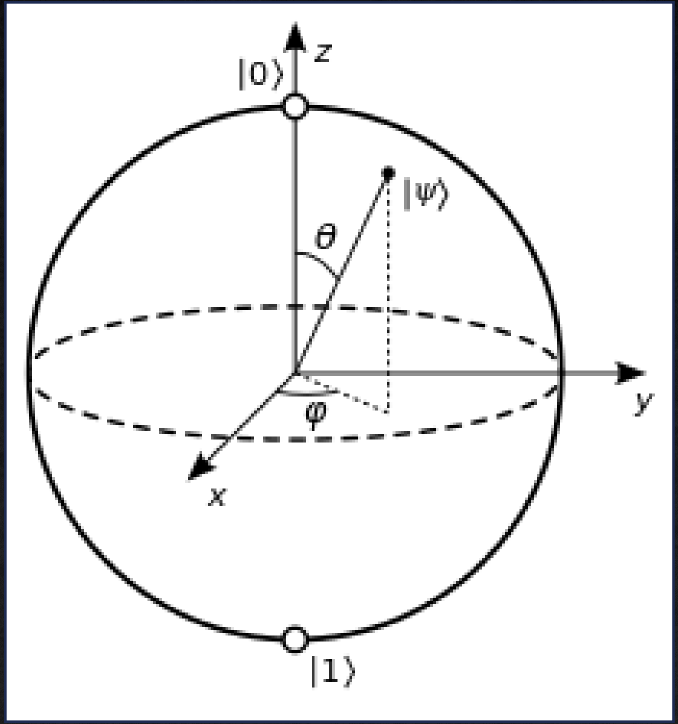
PHYS 6260

Brief overview of CUDA-Q

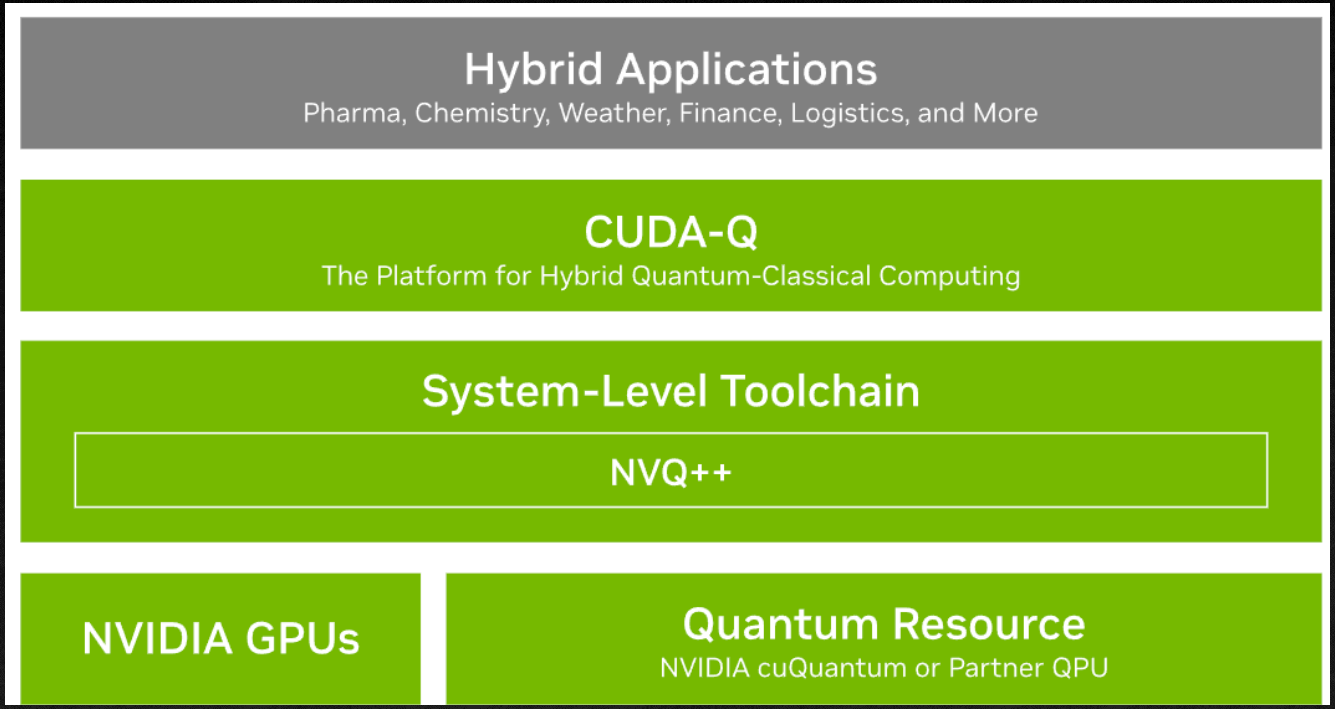
Quantum computing at a glance

- Design quantum circuits with various gates
- Uses bra-ket notation: $|0\rangle = \begin{bmatrix}1\\0\end{bmatrix}, |1\rangle = \begin{bmatrix}0\\1\end{bmatrix}$ basis states
- Instead of 0/1 bits, qubits can be superposition
$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$
- Here α and β are the probability amplitudes and are complex numbers. Their norm is always normalized to 1.
- Multi-qubit states are represented as $|00\rangle, |10\rangle, |101\rangle$, etc
- Qubits can be represented on a "Bloch sphere" showing their probabilities through
$$\alpha = e^{i\delta}\cos\frac{\theta}{2}, \qquad \beta = e^{i(\delta+\phi)}\sin\frac{\theta}{2}$$
- Classical bits would be at the N/S poles
- Qubits can be entangled





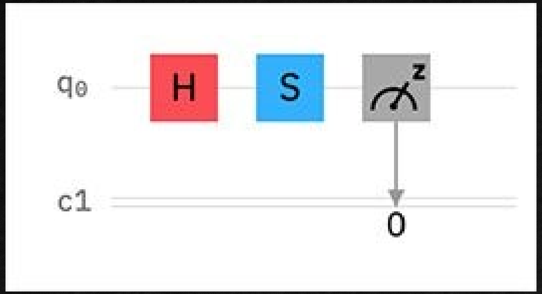
CUDA-Q

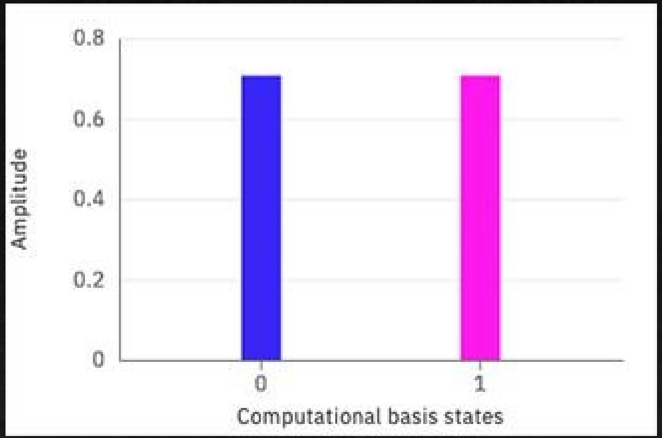


- 2021: Nvidia releases cuQuantum – an SDK of optimized libraries and tools for quantum computing workflows, e.g. quantum circuit simulations
- 2022: Nvidia releases CUDA-Q in an early interest program
- 2024: Nvidia releases CUDA-Q to all
- IBM is also highly invested in quantum computing. Google, Amazon, Microsoft, and Intel, also.

Quantum circuit examples

Using IBM's [Quantum Composer]() (going away on May 15th 😭)





This 2-qubit circuit has a state

$$|\psi\rangle = (\ |00\rangle + |01\rangle + |10\rangle - |11\rangle)/2$$

Operator	Gate(s)		Matrix
Pauli-X (X)	X		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	Y		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	Z		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	H		$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	S		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	T		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)	Z		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)			$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$

Applications

- Most applications are simulating quantum circuits and associated algorithms
- The benefit of SDKs like CUDA-Q is that they allow you to develop code that can run on either CPUs, GPUs, or QPUs

- However, one application caught my eye – Hybrid Quantum Neural Networks
- Here we have a quantum circuit in place of one or multiple traditional NN layers
- This example uses a 1-qubit circuit to compute the gradients

- I think the combination of ML and quantum computing might be the most impactful in the near-term

Applications

1. **Enhanced performance:** HQNNs have the potential to outperform classical neural networks in certain tasks, such as pattern recognition, optimization, and data classification, due to the inherent parallelism and superposition properties of quantum computing.
2. **Limited data availability:** HQNNs have shown promise in scenarios where training data is limited, as they can leverage the quantum circuit's ability to represent complex functions with fewer parameters compared to classical neural networks.
3. **Binary classification:** HQNNs have been successfully applied to binary classification tasks, demonstrating competitive performance compared to classical neural networks on various datasets.

Applications

4. **Financial predictions:** HQNNs have been used for financial predictions, such as predicting stock prices, by transforming financial time series data into a sequence of density matrices and then using a deep quantum network to predict future values.
5. **Medical diagnostics:** HQNNs have been employed in medical diagnostics, particularly for tasks like cancer identification, where accurate and reliable predictions are crucial.
6. **Noisy datasets:** HQNNs have been applied to improve binary classification models for noisy datasets, which are prevalent in financial datasets, by leveraging the capabilities of quantum machine learning frameworks.