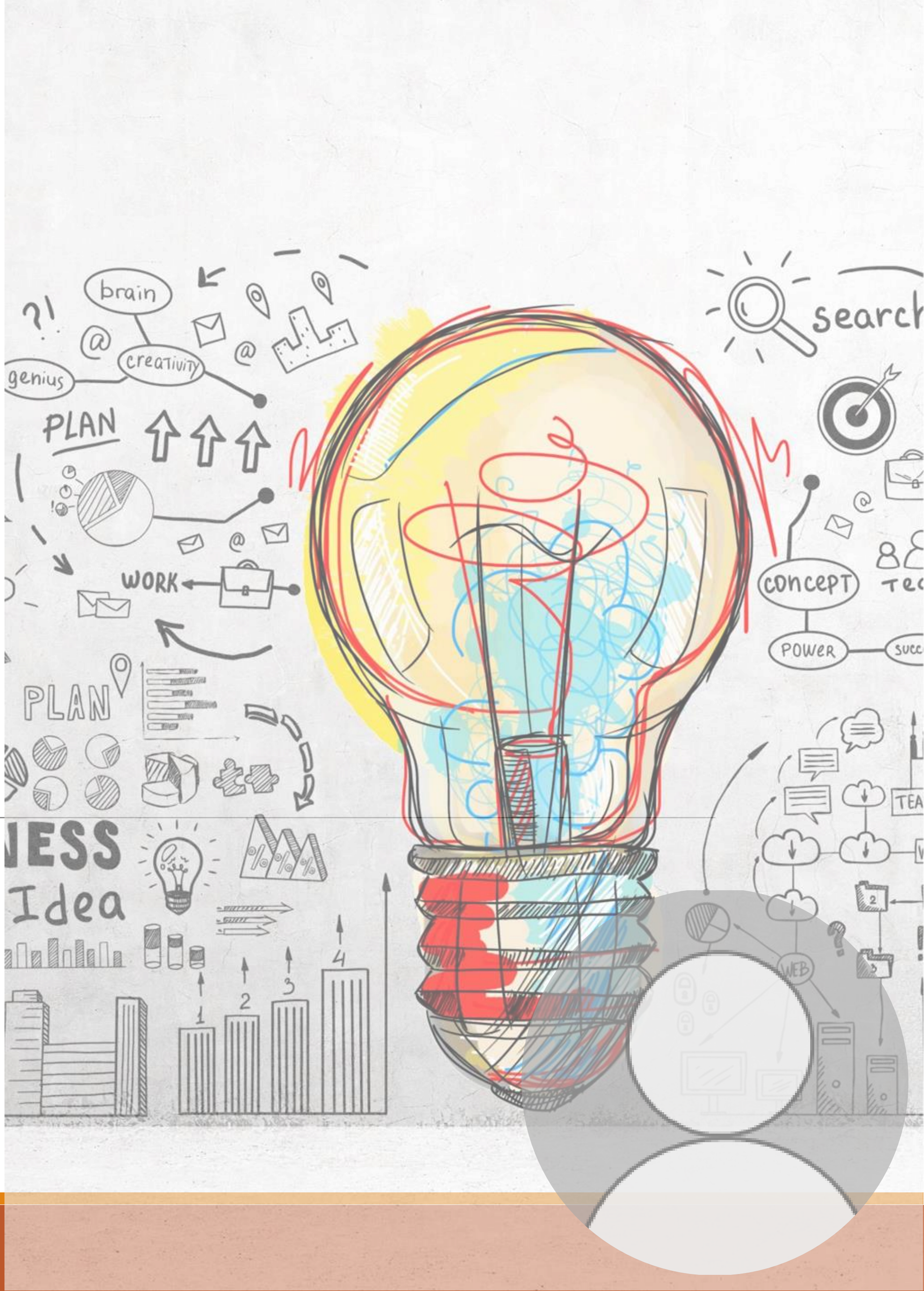
Variational Quantum Algorithms (VQA)

and its application in Quantum Neural Networks (QNNs)



Team 10
AQC III - Final Project

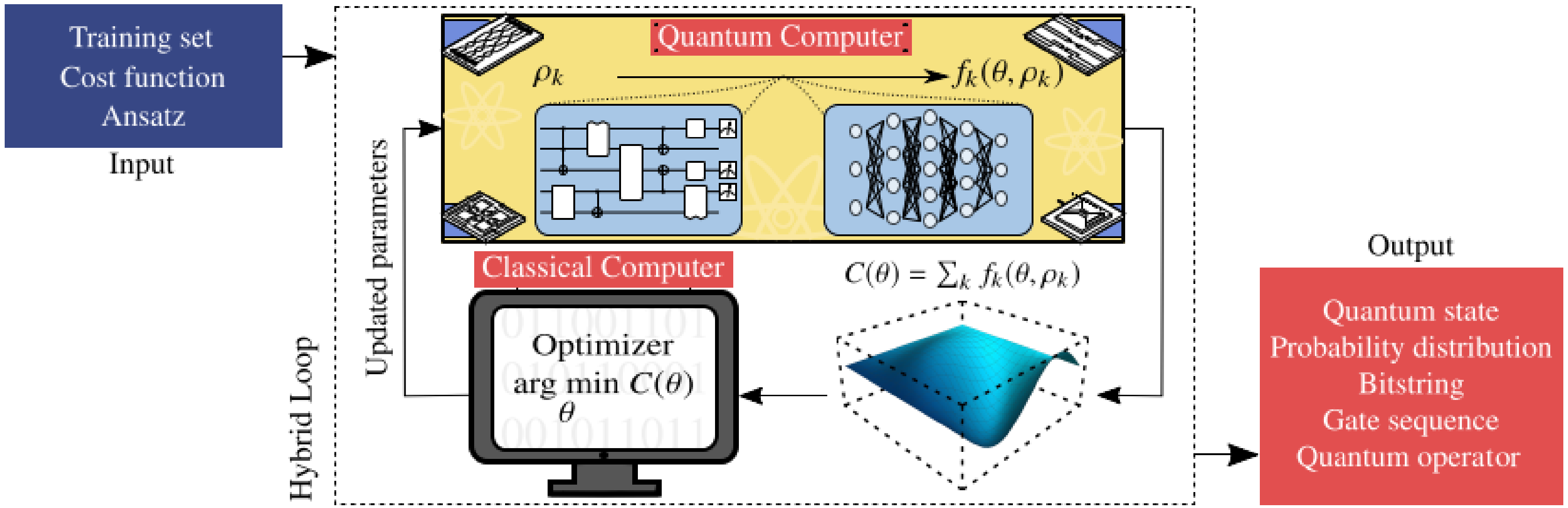
Supervisor
Professor Pramey Upadhyaya

Introduction

- **Problem Statement:** Currently, quantum systems are constrained by number of qubits and noise; limiting circuit depth
- **VQAs** are a strategy that take advantage of current **N**oisy **I**ntermediate-**S**cale **Q**uantum (NISQ) computers with a classical optimizer to address these constraints

The main elements of most VQAs consist of:

- Cost Functions
- Ansatzes
- Gradients
- Optimizers



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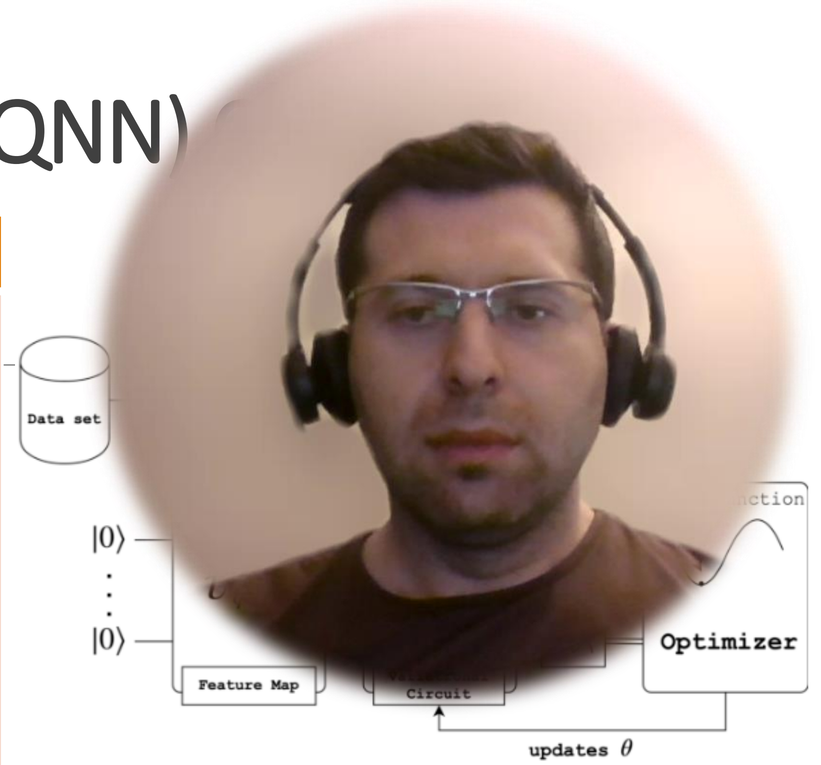
VQA Methods in Quantum Neural Network (QNN)

	Classical Neural Network	Quantum Neural Network
1. Modeling	$f(x,\theta)$ $= f\left(..f\left(w_{ij}^2 . f(w_{ij}^1 . x_j + b_1)\right)...+ b_n\right)$, where $\theta = Wx + b$,	a) **Ansatz**: Amplitude encoding (kernel methods), Block-encoding $U(\theta) = U_L(\theta_L)U_{L-1}(\theta_{L-1})...U_1(\theta_1)$ (Variational circuit) $U_i(\theta_i)$: $R_x(\theta), R_y(\theta), R_z(\theta), CNOT, CZ,$ where: θ *is Rotation angles* $V(x) = V_M(x_M)V_{M-1}(x_{M-1})...V_1(x_1)$ (Feature Map) b) **Measurement of Observables**: Expectation values, Rotation angles estimation $M = \langle\psi_0\|V^\dagger(x^{(i)})U^\dagger(\theta)x^\dagger x U(\theta)V(x)\|\psi_0\rangle$
2. Optimization	$C(\theta) = \sum_x \|f(x;\theta) - y\|^2$ **Cost function**: Mean square error $\theta^{t+1} = \theta^t - \gamma\nabla_\theta C$ **Optimizer**: Gradient-descent with learning rate γ	$C(\theta) = \sum_i\left[y^{(i)} - \langle\psi_0\|V^\dagger(x^{(i)})U^\dagger(\theta)\, A\, U(\theta)V(x^{(i)})\|\psi_0\rangle\right]^2$ **Cost function**: Mean square error $\theta^{t+1} = \theta^t - \gamma\nabla_\theta C$ **Optimizer**: Gradient-descent with learning rate γ



QNN Libraries

Qiskit

TensorFlow

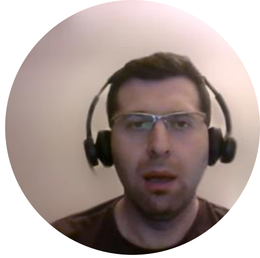
PENNYLANE

PyTorch

Implementation of QNN Classifier

GitHub Link: https://github.com/imanzabet/AQC/blob/main/Qiskit_QNN_Classifier.ipynb

VQA Methods in Quantum Neural Network (QNN) Classifier



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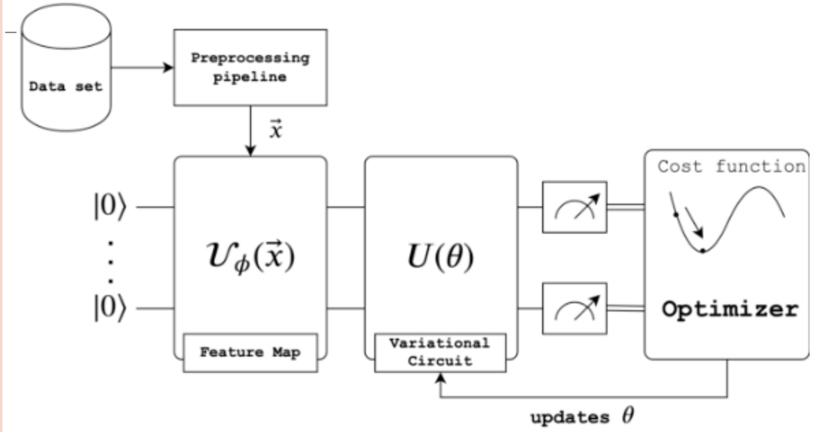

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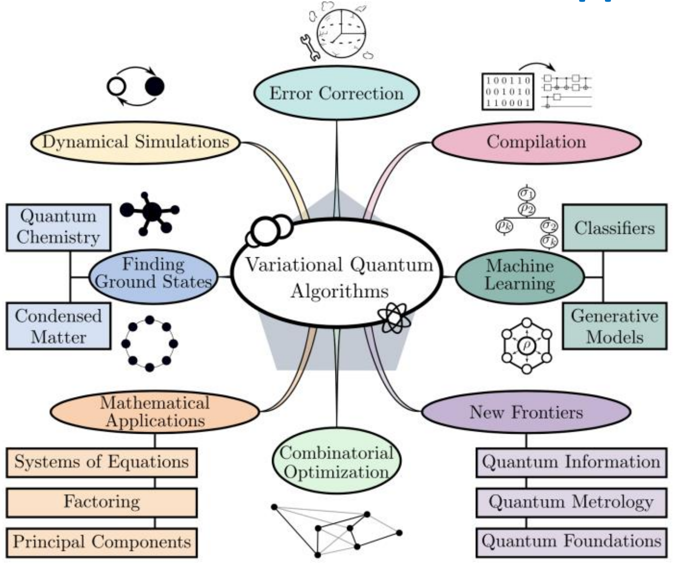
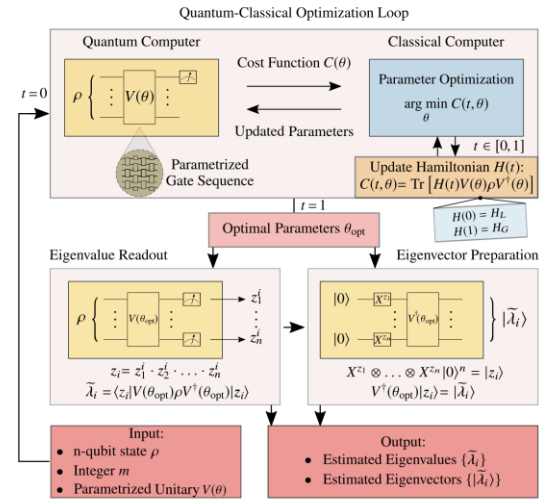
Core ideas and methods involved: applications & challenges/solutions

Applications



VQSE: Condensed Matter Physics



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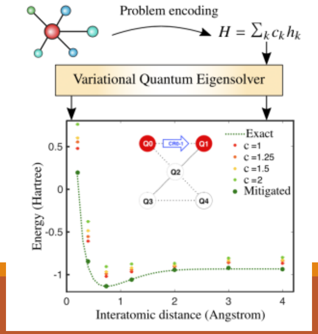
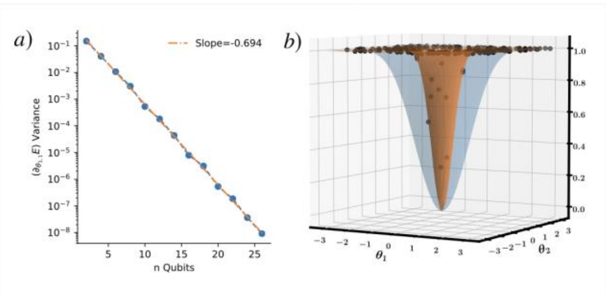
Quantum Chemistry: Finding Ground & Excited States

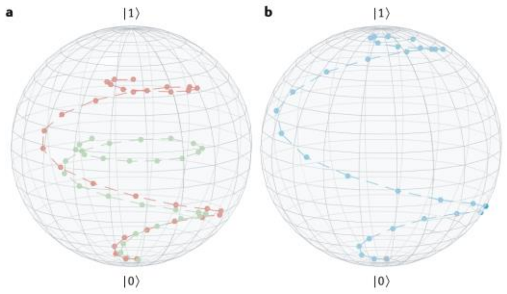


Challenges/Solutions

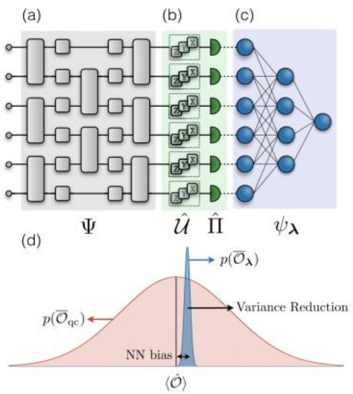
Trainability: Barren plateaus



Accuracy: Quantum Error Mitigation



Efficiency: Expectation Value Estimation



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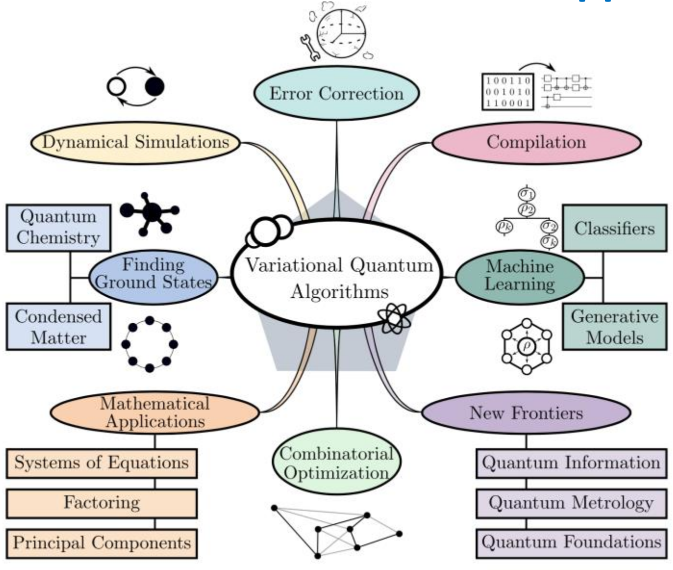

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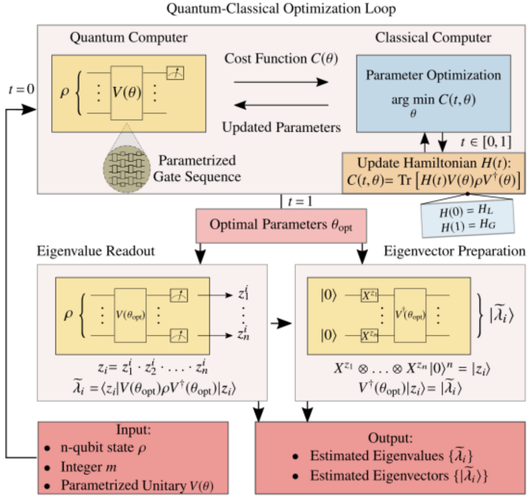

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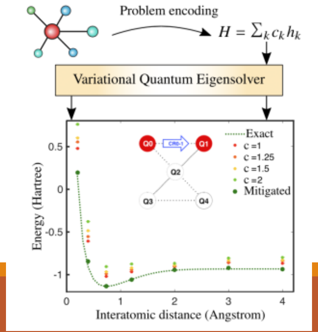

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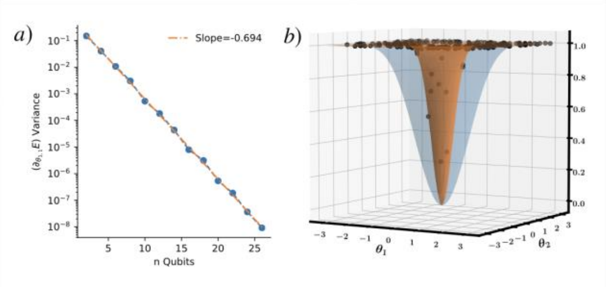

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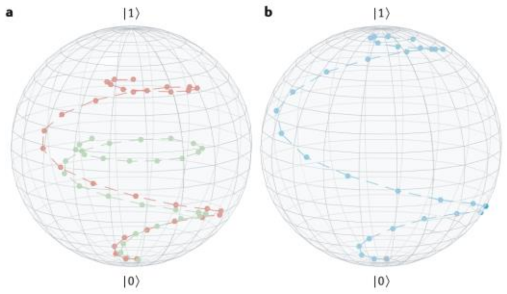

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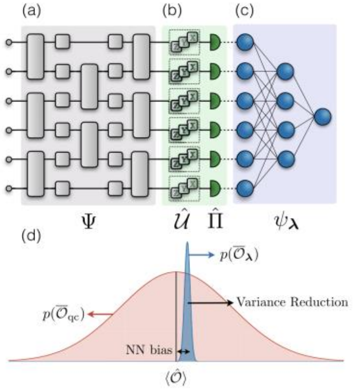

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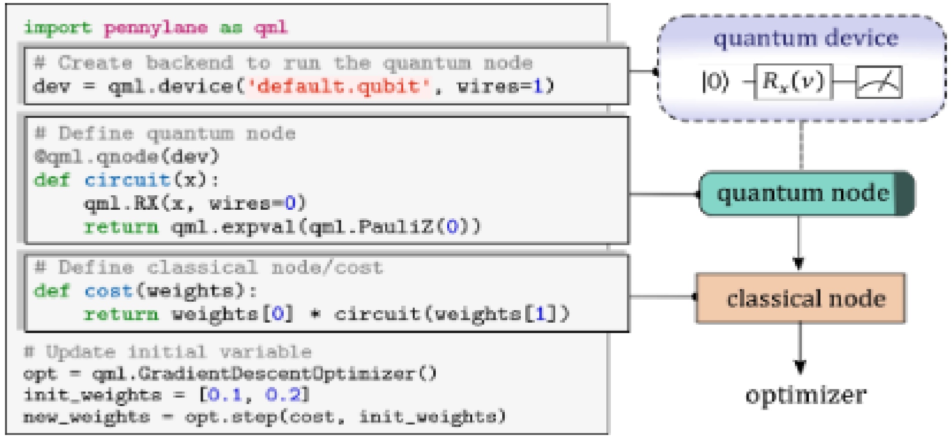

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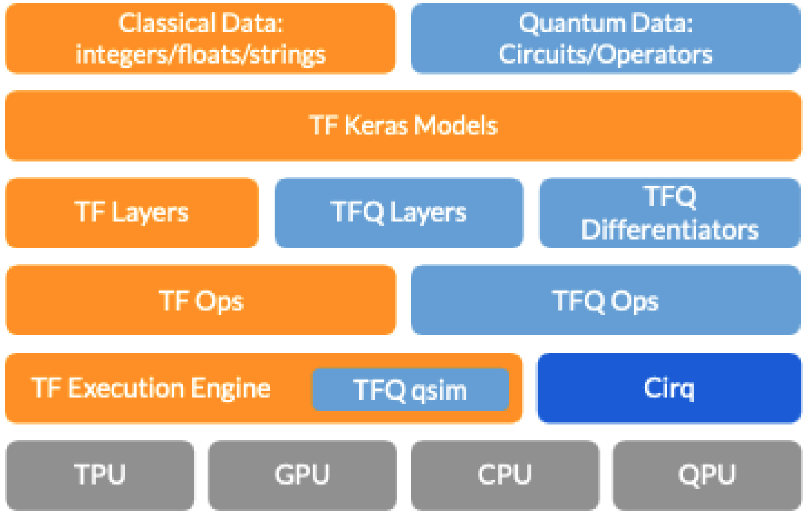

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Ongoing Research

- Chemistry and Material Science
- Nuclear and Particle Physics
- Optimization and Machine Learning
  - Quantum Neural Networks vs Classical

Giving Greater Access to QNNS:

Pennylane:

https://pennylane.ai/

Tensorflow Quantum:

https://www.tensorflow.org/quantum

THANK YOU