Quantum Machine Learning in HEP with `Qibo`

PyHEP 2024

Matteo Robbiati[†] on behalf of the Qibo team[‡]

3 July 2023

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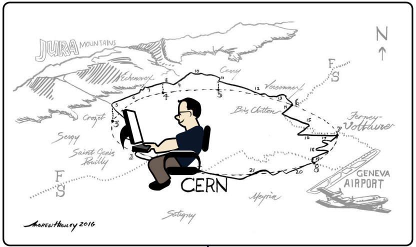
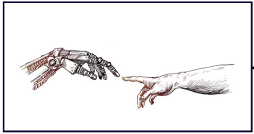
Quantum Computing for HEP

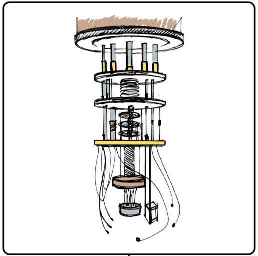
High Energy Physics



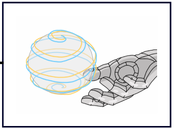
- Plenty of data to analyze
- Need for technological development



Quantum computers



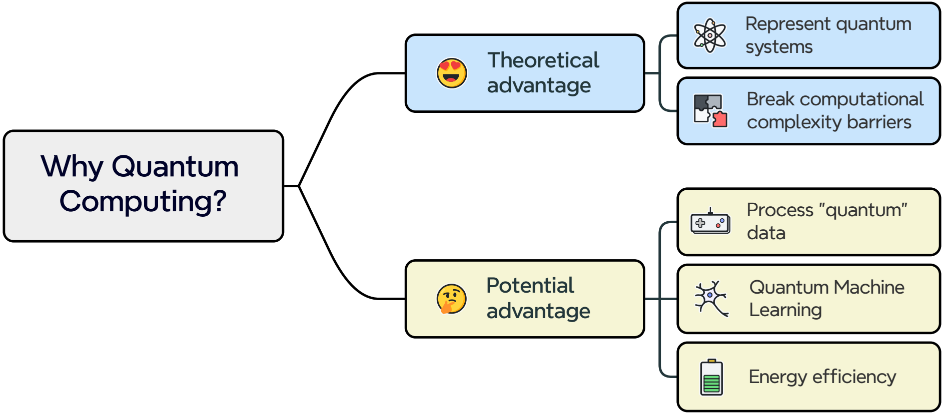
- Computational boost (problem specific)
- Noise and limited resources
  - Simulation
  - Control
  - Calibration



« For HEP! »

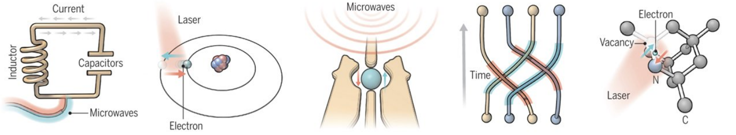
Quantum Computing in a nutshell

A quite general “why?”



Gate based quantum computing

1. classical bits are replaced by **qubits** $|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$ (quantum states).



Superconducting loops
A resistance-free current oscillates back and forth around a circuit loop. An injected microwave signal excites the current into superposition states.

Trapped ions
Electrically charged atoms, or ions, have quantum energies that depend on the location of electrons. Tuned lasers cool and trap the ions, and put them in superposition states.

Silicon quantum dots
These "artificial atoms" are made by adding an electron to a small piece of pure silicon. Microwaves control the electron's quantum state.

Topological qubits
Quasiparticles can be seen in the behavior of electrons channeled through semiconductor structures. Their braided paths can encode quantum information.

Diamond vacancies
A nitrogen atom and a vacancy add an electron to a diamond lattice. Its quantum spin state, along with those of nearby carbon nuclei, can be controlled with light.

Gate based quantum computing

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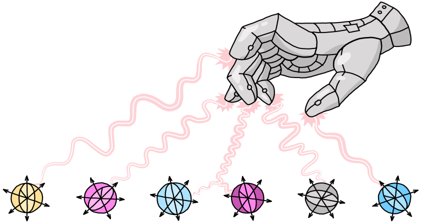
2. we can manipulate the qubit state applying **gates**: $|\psi'\rangle = \mathcal{U}(\boldsymbol{\theta})|\psi\rangle$.
   Typically we use 1-qubit and 2-qubits gates!



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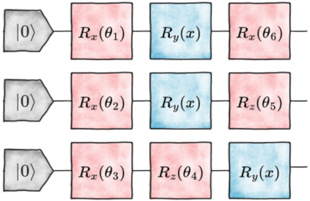
3. combine together gates to build **quantum circuits**;



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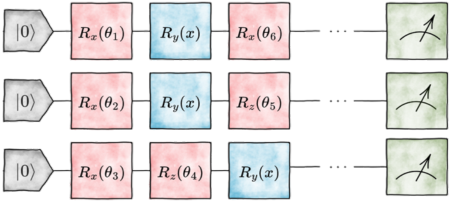
3. combine together gates to build **quantum circuits**;
4. to access the information we need to measure the system.



Example 1: preparing entangled states

With quantum computing, we introduce new tools.

- prepare a quantum state in the computational zero $|0\rangle$;
- we can prepare superposition:

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \quad \text{with} \quad H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \; |0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \; |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix};$$

- let's apply a controlled-NOT (CNOT) gate on a second qubit prepared in $|0\rangle$:

$$\mathrm{CNOT}\Bigg(\underbrace{\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)}_{\text{control}} \otimes |0\rangle\Bigg) = \frac{1}{\sqrt{2}}(|00\rangle + \mathrm{NOT}_{\mathrm{targ}}|10\rangle) = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle).$$

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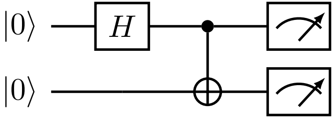
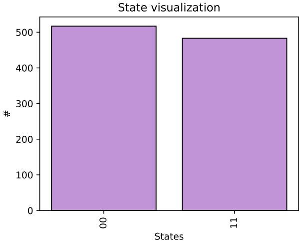
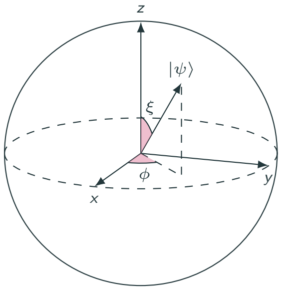


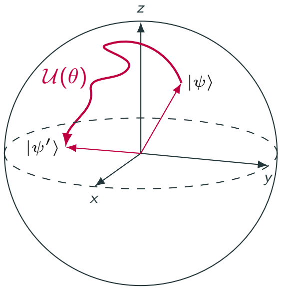


Parametric gates prepare variational quantum states

- Among the gates, parametric ones can be useful!
- Let's consider a single qubit system:

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \qquad \text{with} \qquad \alpha = \cos\frac{\theta}{2}, \quad \beta = e^{i\phi}\sin\frac{\theta}{2}.$$



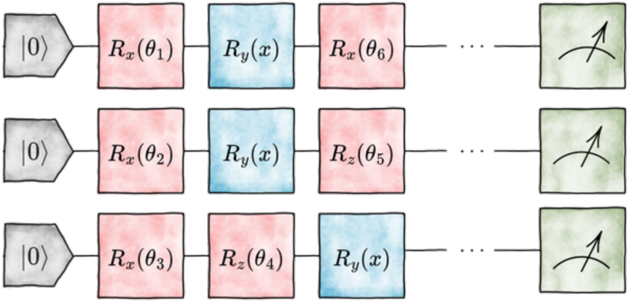


We can use as parametric gates the rotation around the axis of the block sphere:

$$R_k(\theta) = \exp\left[-i\theta\sigma_k\right], \qquad \text{with} \qquad \sigma_k \in \{I, \sigma_x, \sigma_y, \sigma_z\}.$$

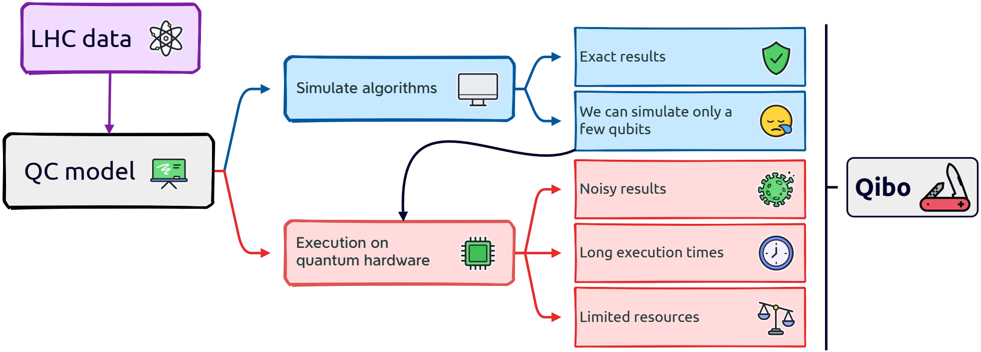
Parametric quantum circuits

Parametric gates can be used to build parametric quantum circuits.

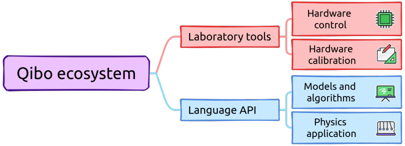


Qibo 0.2.8

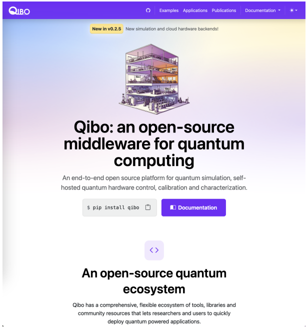
What is needed for doing quantum computing?



Qibo is an **open-source** hybrid quantum operating system for self-hosted quantum computers.

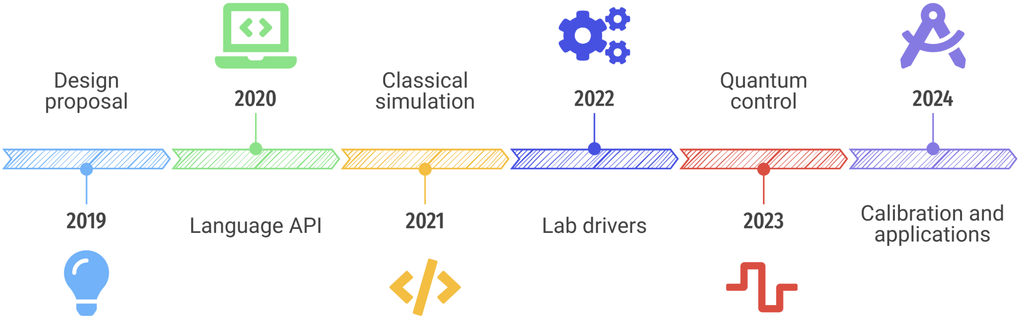


1. Fully open-source and community driven.
2. Modular layout design with possibility of adding:
   - new backends for simulation,
   - new platforms for hardware control,
   - new drivers for control electronics.
3. Supported by documentation and tests/CI on quantum hardware.



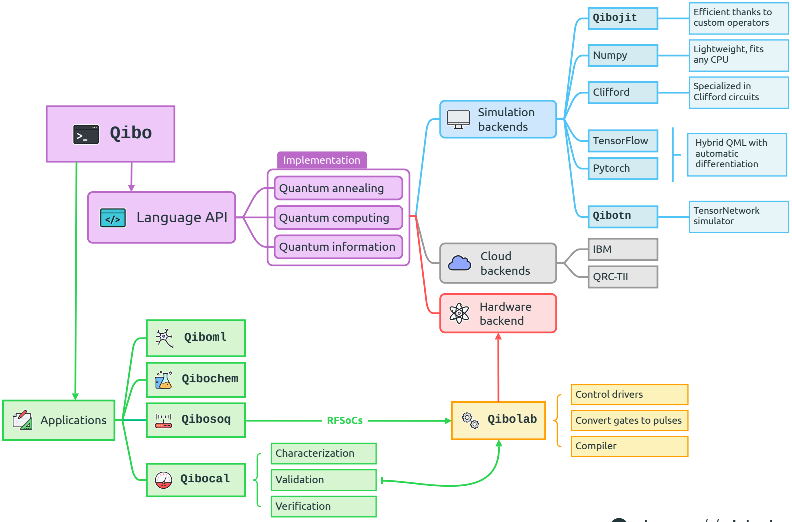
https://qibo.science

The Qibo timeline



An open source and full-stack framework for QC

arXiv:2308.06313



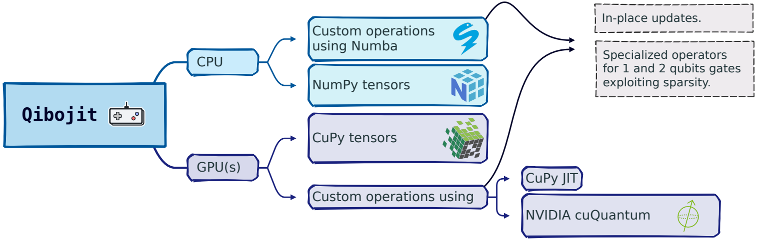
https://github.com/qiboteam

State vector simulation solves:

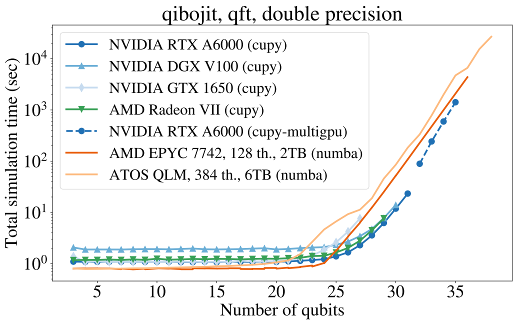
$$\psi'(\sigma_1, \ldots, \sigma_n) = \sum_{\boldsymbol{\tau}'} G(\boldsymbol{\tau}, \boldsymbol{\tau}')\psi(\sigma_1, \ldots, \boldsymbol{\tau}', \ldots, \sigma_n)$$

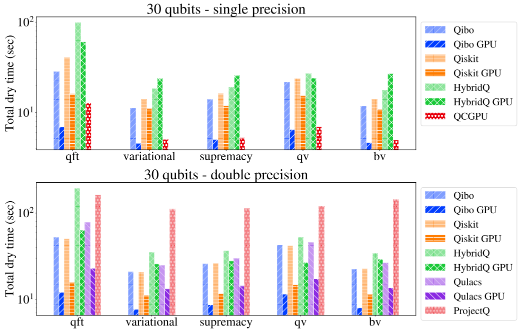
The number of operations scales exponentially with the number of qubits.

Qibo uses just-in-time technology and hardware acceleration:



Through its modularity, `Qibo` allows execution of the same high level language onto different classical hardware accellerators.



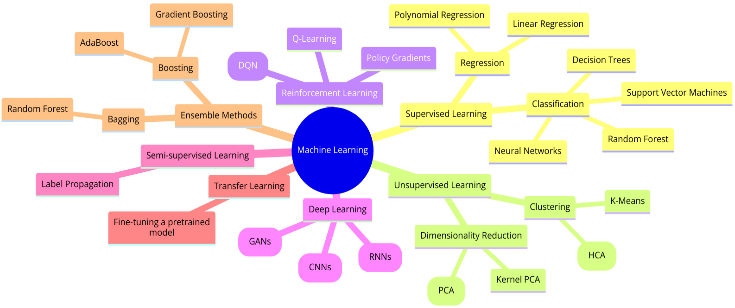


We reach satisfying performances thanks to custom operators and in-place updates of the statevector.

Quantum Machine Learning

Classical Machine Learning

I asked ChatGPT to give me a comprehensive diagram of Machine Learning (ML) models.



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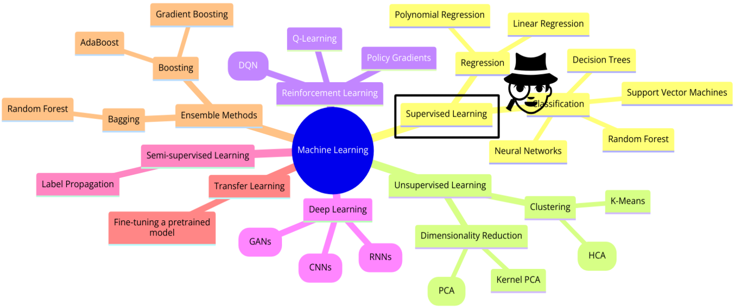
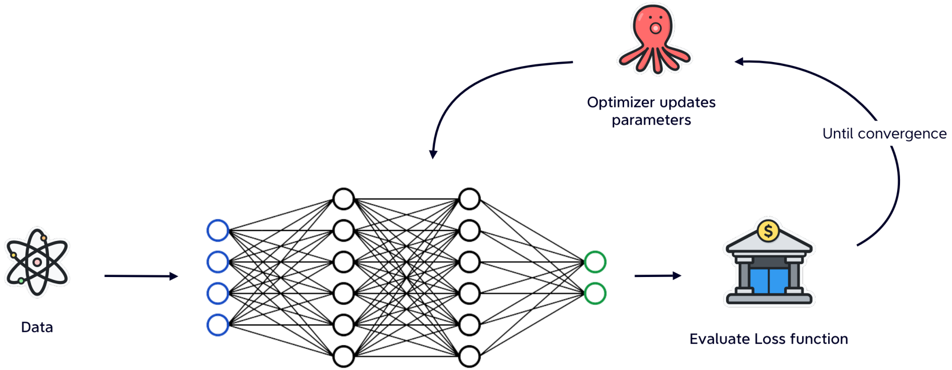


Focusing on the supervised ML!

- we aim to know some hidden law between two variables: $\boldsymbol{y} = f(\boldsymbol{x})$;
- we define a parameteric model which returns $\boldsymbol{y}_{\mathrm{est}} = f_{\mathrm{est}}(\boldsymbol{x}; \boldsymbol{\theta})$;
- we define an optimizer, which task is to compute $\operatorname{argmin}_{\boldsymbol{\theta}} \left[J(\boldsymbol{y}_{\mathrm{meas}}, \boldsymbol{y}_{\mathrm{est}}) \right]$.

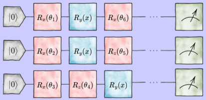
Classical Machine Learning



Machine Learning
$\mathcal{M}$: model;
$\mathcal{O}$: optimizer;
$\mathcal{J}$: loss function.
(x, y): data

Quantum Computation
$\mathcal{Q}$: qubits;
$\mathcal{S}$: superposition;
$\mathcal{E}$: entanglement.

Circuit execution



Expected values
$y_{est} \equiv \langle q_f | \hat{O} | q_f \rangle$

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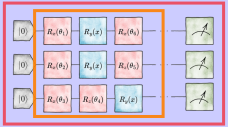

Quantum Machine Learning!

Optimizer $\mathcal{O}$
Hybrid-strategy

Machine Learning
$\mathcal{M}$: model;
$\mathcal{O}$: optimizer;
$\mathcal{J}$: loss function.
(x, y): data

loss function $\mathcal{J}$
$\mathcal{J}(y_{meas}, y_{est})$

Expected values
$y_{est} \equiv \langle q_f | \hat{O} | q_f \rangle$

Quantum Computation
$\mathcal{Q}$: qubits;
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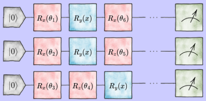
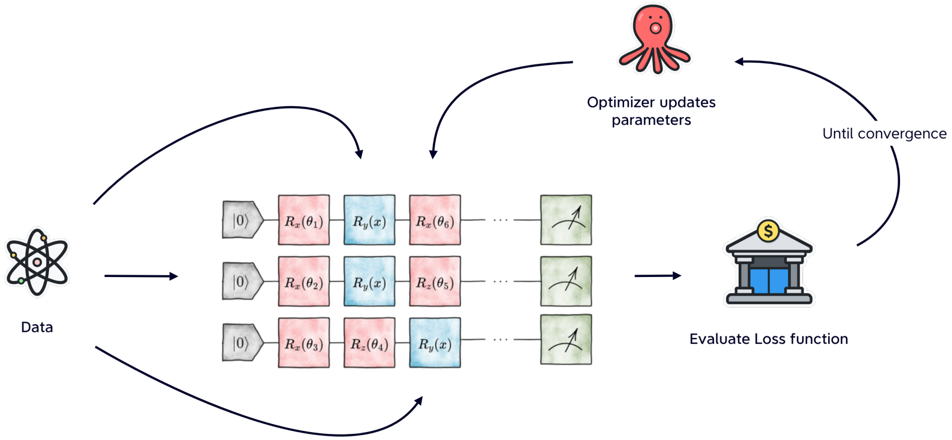
Circuit execution



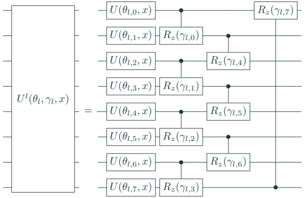

Optimizer updates parameters
Until convergence
$|0\rangle$
$R_x(\theta_1)$
$R_y(x)$
$R_x(\theta_6)$
$|0\rangle$
$R_x(\theta_2)$
$R_y(x)$
$R_z(\theta_5)$
$|0\rangle$
$R_x(\theta_3)$
$R_z(\theta_4)$
$R_y(x)$
Data
Evaluate Loss function

 arXiv:2011.13934

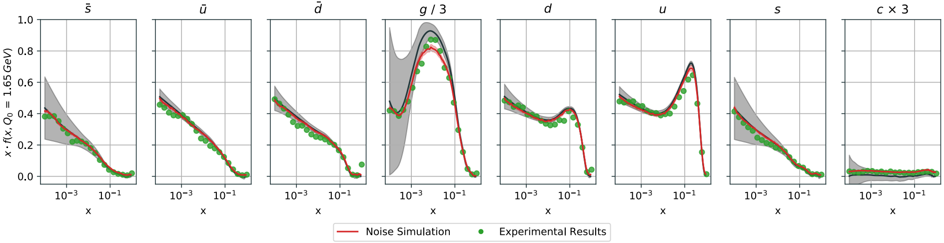
We parametrize **Parton Distribution Functions** with multi-qubit variational quantum circuits:

1. Define a quantum circuit: $\mathcal{U}(\theta, x)|0\rangle^{\otimes n} = |\psi(\theta, x)\rangle$
2. $U_w(\alpha, x) = R_z(\alpha_3 \log(x) + \alpha_4) R_y(\alpha_1 \log(x) + \alpha_2)$
3. Using $z_i(\theta, x) = \langle \psi(\theta, x)|Z_i|\psi(\theta, x)\rangle$:

$$\mathrm{qPDF}_i(x, Q_0, \theta) = \frac{1 - z_i(\theta, x)}{1 + z_i(\theta, x)}.$$



Results from **classical quantum simulation and hardware execution** (IBM) are **promising**:



PDF fit on chip

arXiv:2308.06313

High level API: Qibo

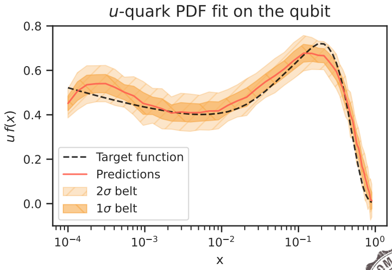
- define **prototypes** and models;
- **simulate** training and noise.

Calibration: Qibocal

- **calibrate** qubits;
- generate **platform configuration**;

Execution: Qibolab

- allocate **calibrated** platform;
- **compile** and **transpile** circuits;
- execute and return **results**.



Parameter	Value
N_{data}	50
N_{shots}	500
MSE	$\sim 10^{-3}$
Electronics	Xilinx ZCU216
Training time	$\sim$ 2h

Some applications

- Multi-variable integration using the qPDF ansatz, arXiv:2303.11346;
- Real-time quantum error mitigation on superconducting devices to improve trainability, arXiv:2303.11346;