Quantum computers for particle theory

Challenges and achievements in the NISQ era

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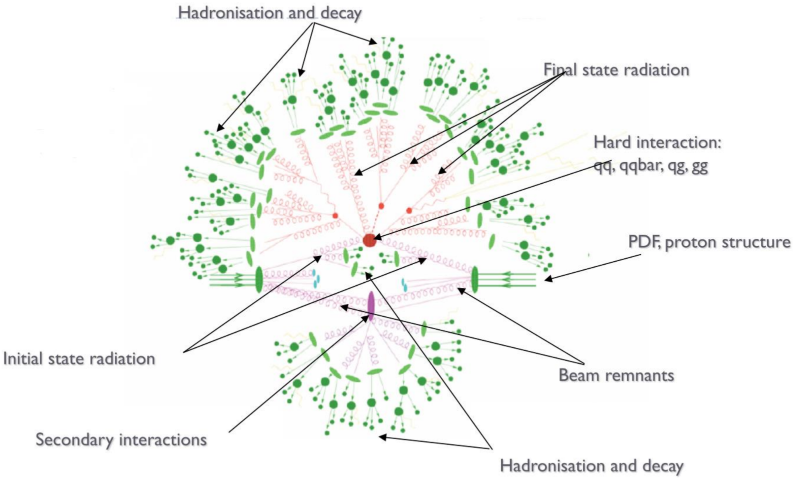
ACAT2024, Stony Brook

HEP challenges for LHC and future colliders

Monte Carlo simulation and data analysis are **intensive** and requires lots of **computing power**.



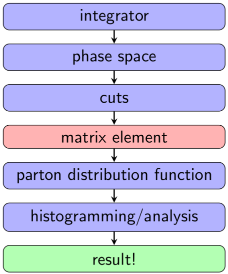
Parton-level Monte Carlo generators

Theoretical predictions in `hep-ph` are based on:

$$\sum_{a,b} \int_{x_{\min}}^{1} dx_1 dx_2 \, |\mathcal{M}_{ab}(\{p_n\})|^2 \, \mathcal{J}_m^n(\{p_n\}) \, f_a(x_1, Q^2) f_b(x_2, Q^2),$$

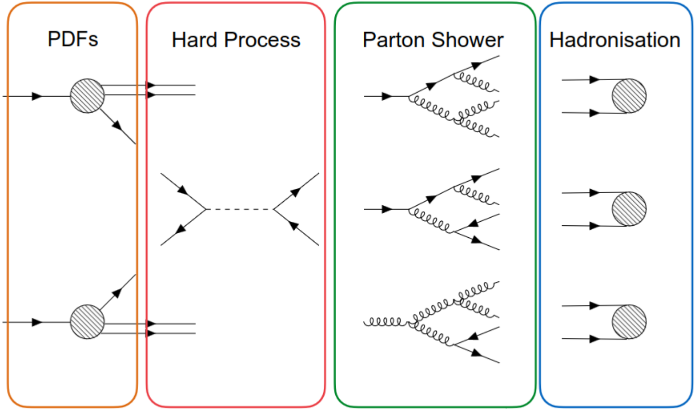
a multi-dimensional integral where:

- $|\mathcal{M}|$ is the matrix element,
- $f_i(x, Q^2)$ are Parton Distribution Functions (PDFs),
- $\{p_n\}$ phase space for n particles,
- $\mathcal{J}_m^n$ jet function for n particles to m.



$\Rightarrow$ **Procedure driven by the integration algorithm.**

Monte Carlo generator pipeline



R&D and adoption of new technologies in HEP

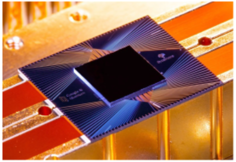
HEP is moving towards new technologies, in particular **hardware accelerators**:

CPU

GPU

FPGA/ASIC

Quantum chip



Moving from **general purpose devices** $\Rightarrow$ **application specific**

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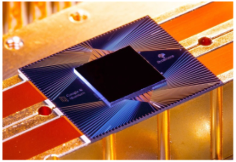
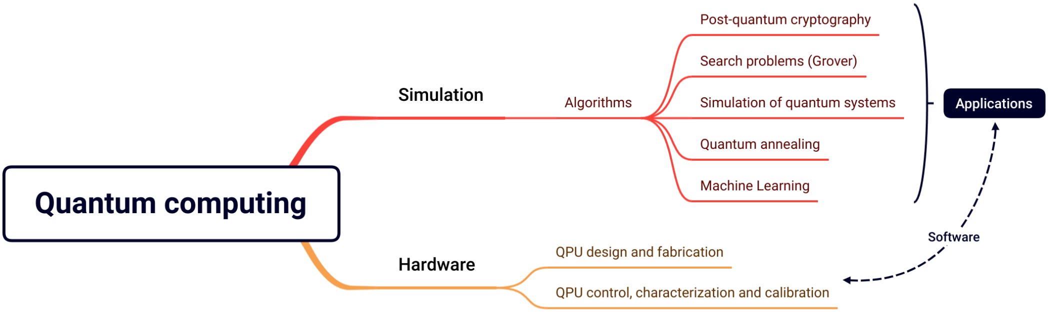
			

Moving from **general purpose devices** $\Rightarrow$ **application specific**

Examples of **initiatives** and institutions involved:

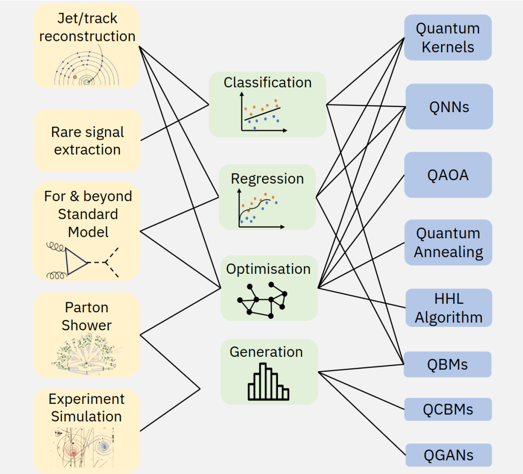
CERN | QUANTUM TECHNOLOGY INITIATIVE INFN BIQUTE

Quantum Computing topics in HEP



The **HEP community** is testing **quantum computing algorithms** in topics related to:

hep-exp	hep-ph	quant-ph
Data analysis	Theoretical modelling	Software / Middleware



QC4HEP WG

Goal:

Replace **classical ML data analysis** methods with variational quantum computing (QML) and observe **advantage** with quantum computing methods.

How?

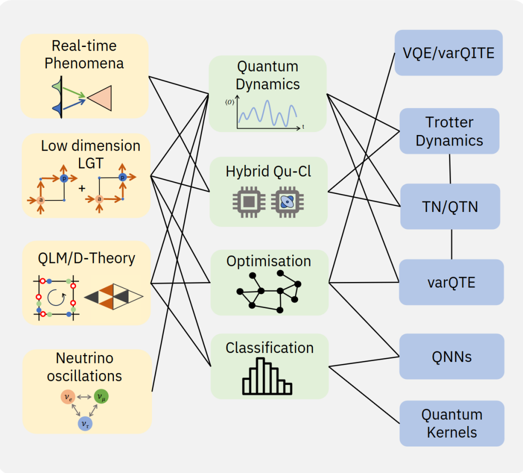
- Developing **variational models** using classical quantum simulation.
- Adapting problems and deploying strategies on **NISQ hardware**.

Goal:

Design **new algorithms** for QFT and Hadronic physics observables, identify **advantage** from quantum computing methods.

How?

- Designing **hybrid quantum-classical** methods using classical quantum simulation.
- Deploying **classical quantum simulation** techniques on HPC infrastructure.



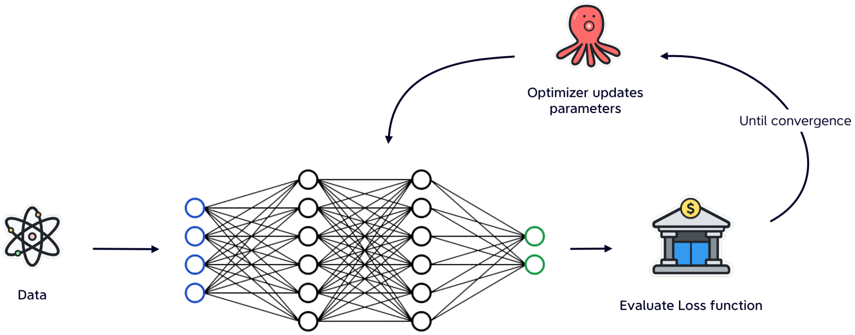
QC4HEP WG

Quantum machine learning

From classical Machine Learning to quantum

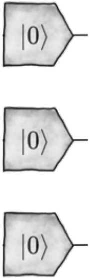
Classical **Machine Learning** solves statistical problems such as data generation, classification, regression, forecasting, etc.

- Aims to know some hidden law between two variables: $\boldsymbol{y} = f(\boldsymbol{x})$;
- Defines a parametric model with returns $\boldsymbol{y}_{\rm est} = f_{\rm est}(\boldsymbol{x};\boldsymbol{\theta})$;
- Defines an optimizer, which task is to compute $\text{argmin}_{\boldsymbol{\theta}}\big[J(\boldsymbol{y}_{\rm meas}, \boldsymbol{y}_{\rm est})\big]$.



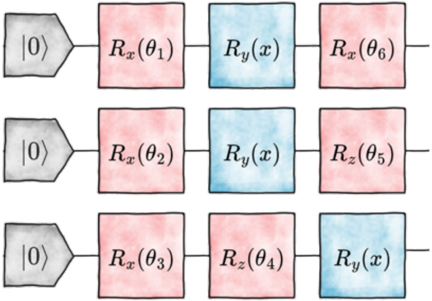
Parametric Quantum Circuits

- Classical bits are replaced by **qubits**: $|q\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle$;



Parametric Quantum Circuits

- Classical bits are replaced by **qubits**: $|q\rangle = \alpha_0 |0\rangle + \alpha_1 |1\rangle$;
- The qubit state is modified by applying **gates** (unitary operators).
  Rotational gates $R_j(\theta) = e^{-i\theta\hat{\sigma}_j}$ are used to build parametric circuits $\mathcal{C}(\boldsymbol{\theta})$;



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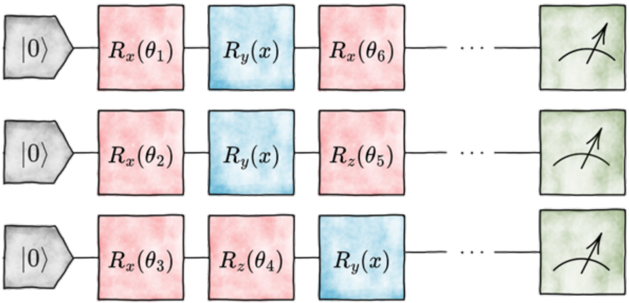
  Rotational gates $R_j(\theta) = e^{-i\theta\hat{\sigma}_j}$ are used to build parametric circuits $\mathcal{C}(\boldsymbol{\theta})$;
- Information is accessed calculating expected values $\mathrm{E}[\hat{O}\,]$ of target observables $\hat{O}$ on the state obtained executing $\mathcal{C}$.



Machine Learning

$\mathcal{M}$: model;

$\mathcal{O}$: optimizer;

$\mathcal{J}$: loss function.

(x, y): data

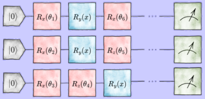
Quantum Computation

$\mathcal{Q}$: qubits;

$\mathcal{S}$: superposition;

$\mathcal{E}$: entanglement.

VQC execution



Expected values

$y_{est} \equiv \langle q_f | B | q_f \rangle$

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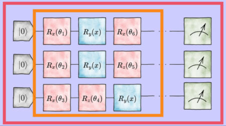

Quantum Machine Learning

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
$y_{est} \equiv \langle q_f | B | q_f \rangle$

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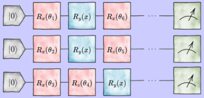
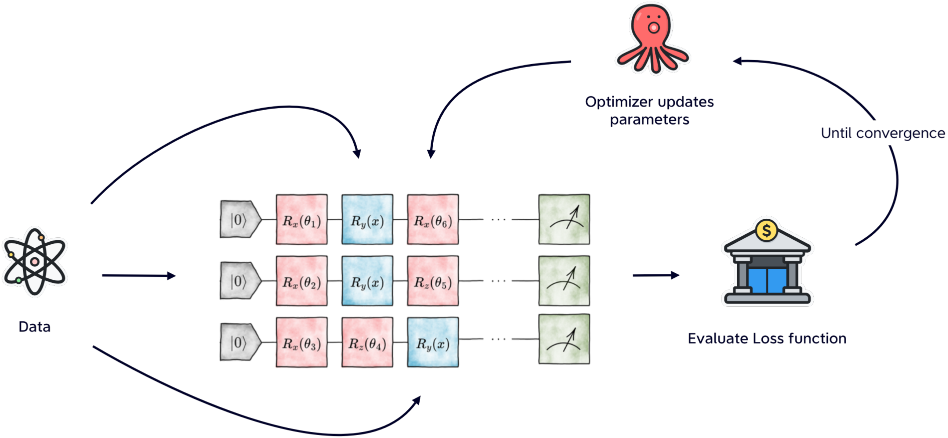
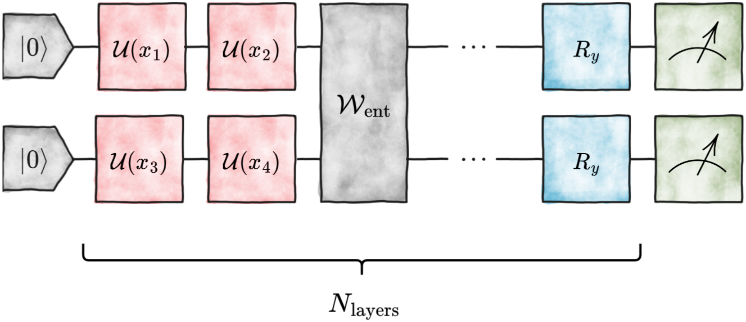
VQC execution



From ML to QML

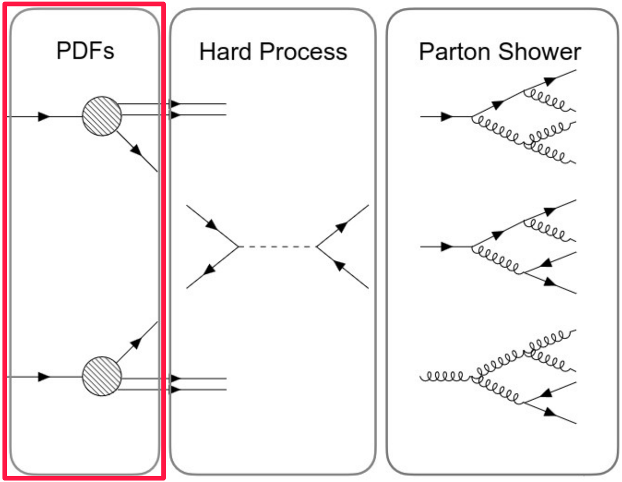


We define an uploading channel $U(x;\boldsymbol{\theta})$, and we repeat the uploading N times.



It has been proved this approach is equivalent to approximate a function with an N-term Fourier Series.

Example 1: Parton Distribution Functions



Parton distribution functions (Machine Learning)

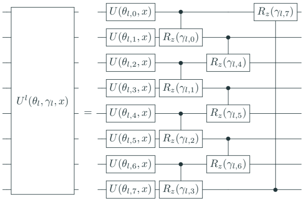
Determination of parton distribution functions

arXiv:2011.13934

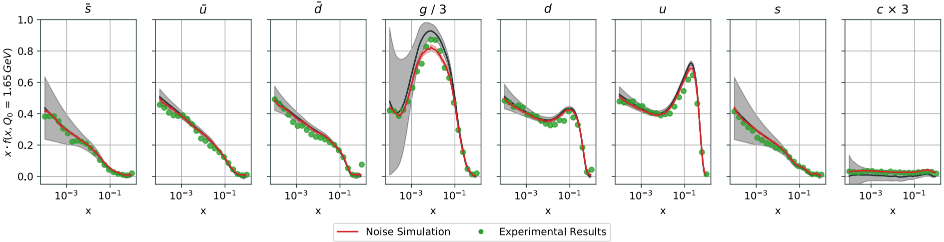
We parametrize **Parton Distribution Functions** with multi-qubit variational quantum circuits:

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 $z_i(\theta, x) = \langle\psi(\theta, x)|Z_i|\psi(\theta, x)\rangle$:

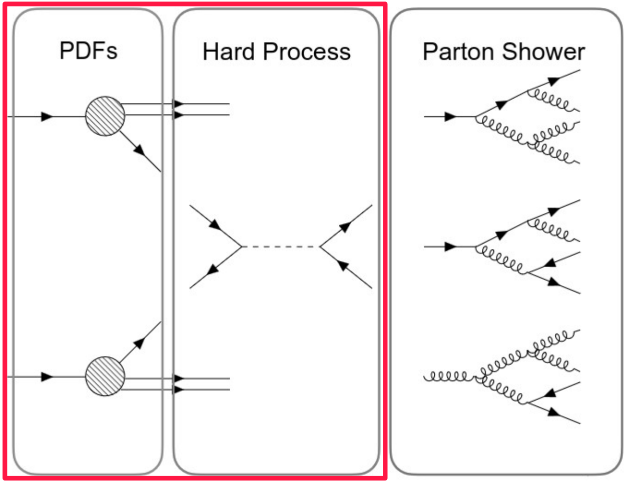
$$\text{qPDF}_i(x, Q_0, \theta) = \frac{1 - z_i(\theta, x)}{1 + z_i(\theta, x)}.$$



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



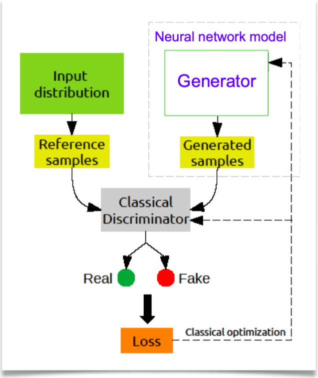
Example 2: Event generation



Event generation

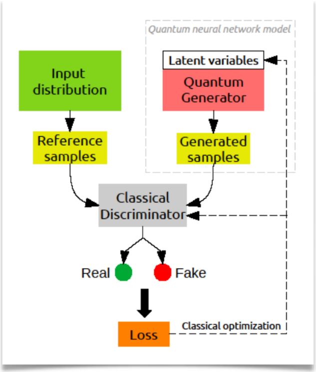
Train with a **small dataset**, use **unsupervised machine learning models** to learn the underlying distribution and generate for free a much larger dataset.

Classical setup:

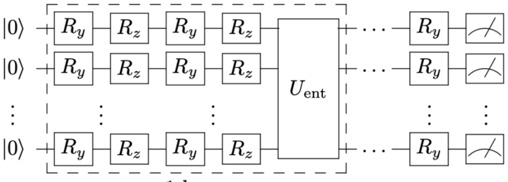


Only the generator becomes quantum

Hybrid quantum-classical setup:



Quantum generator: a series of quantum layers with rotation and entanglement gates



1 component = 1 qubit

$$\boldsymbol{x} = \left(-\left\langle\sigma_z^1\right\rangle, -\left\langle\sigma_z^2\right\rangle, \ldots, -\left\langle\sigma_z^n\right\rangle\right)$$

Style-based approach

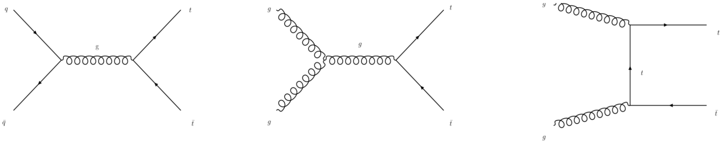
the noise is inserted in **every gate and not only in the initial quantum state**

$$R_{y,z}^{l,m}\left(\boldsymbol{\phi_g}, \boldsymbol{z}\right) = R_{y,z}\left(\phi_g^{(l)} z^{(m)} + \phi_g^{(l-1)}\right)$$

Reminiscent of the reuploading scheme

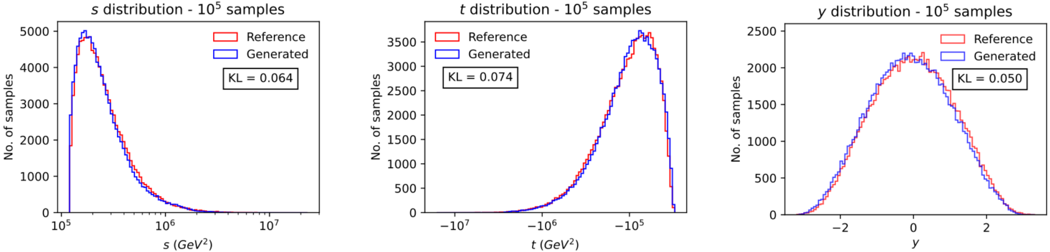
A. Pérez-Salinas, et al., *Quantum* **4**, 226 (2020)

Testing the style-qGAN with real data: proton-proton collision $pp \to t\bar{t}$



Training and reference samples for **Mandelstam variables** (s, t) and rapidity y generated with MadGraph5_aMC@NLO.

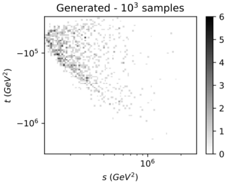
Simulation results: 3 qubits, 2 layers, 100 bins

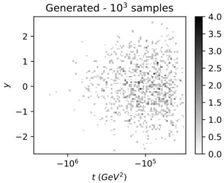


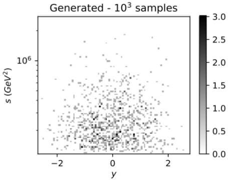
- Access constraints to *ionQ*: test limited to 1000 samples only

Very similar results:
implementation largely hardware-independent

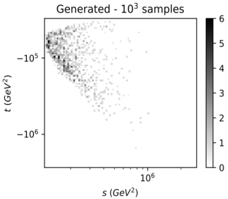
ionQ samples:

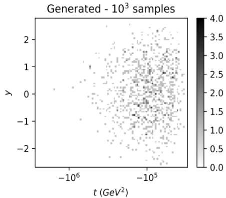


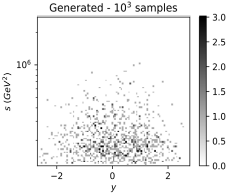




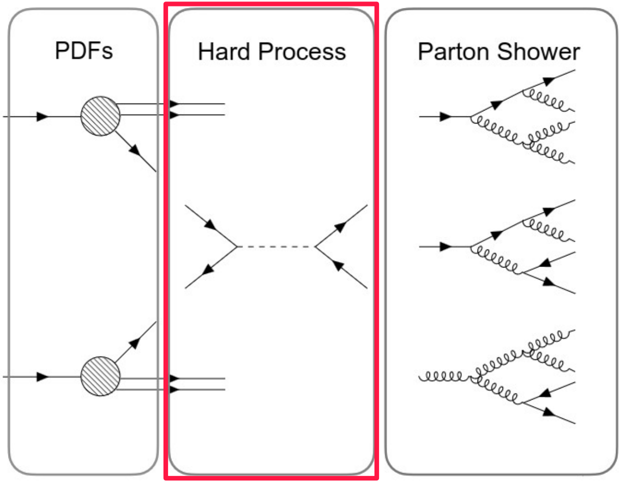
IBM Q samples:





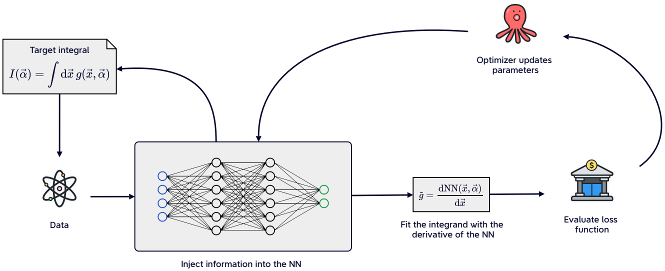


Example 3: Monte Carlo Integration / Sampling

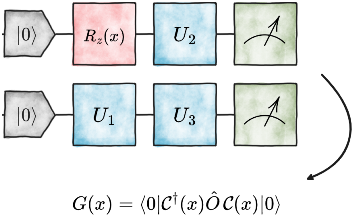


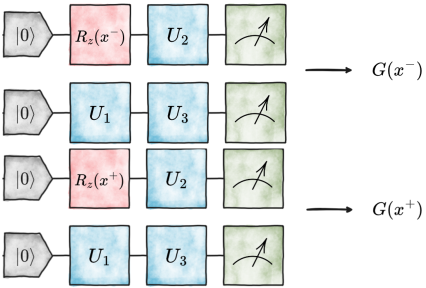
Monte Carlo Integration

Multi-variable integrals using Neural Networks:



- both NN and dNN are models of the integral and integrand respectively;
- once trained, the NN can be called with any combination of data and parameters. Monte Carlo Integration (MCI), instead, has to be recomputed every time;
- in the INN is the integrand to be approximated, instead of the integral (as in MCI), swaps **variance** for approximation error.





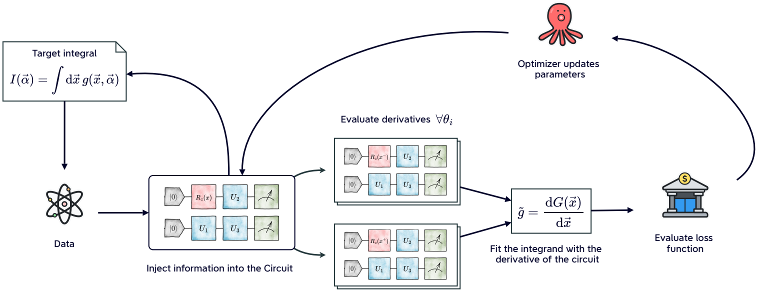
Considering the unitary $\mathcal{U}(x) = e^{-ixU}$ affected by one parameter x, if the hermitian generator U has at most two eigenvalues $\pm r$, an exact estimator of $\partial_x G$ is:

$$\partial_x G = r\left[G(x^+) - G(x^-)\right].$$

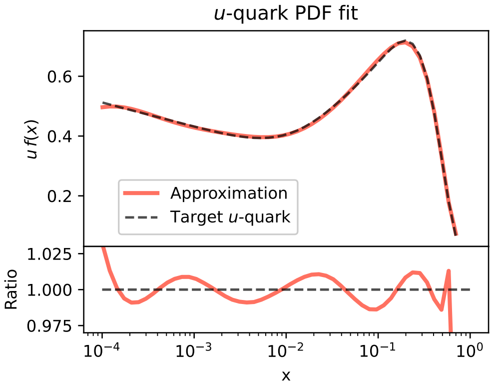
Where $x^{\pm} = x \pm s$ and, considering rotational gates, we have $s = \pi/2$ and $r = 1/2$.

At this point, we know that:

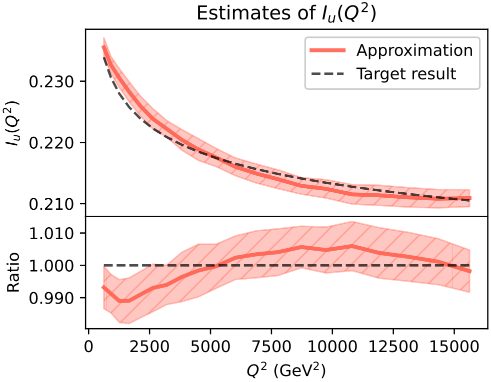
1. **variables** can be **injected** into a quantum circuit as rotational angles;
2. the same circuit architecture $\mathcal{C}$ can be used to compute **both** the estimator and its derivatives.



If independent variables, $\frac{\mathrm{d}G(\boldsymbol{x})}{\mathrm{d}\boldsymbol{x}}$ is obtained by summing all PSR contributions.



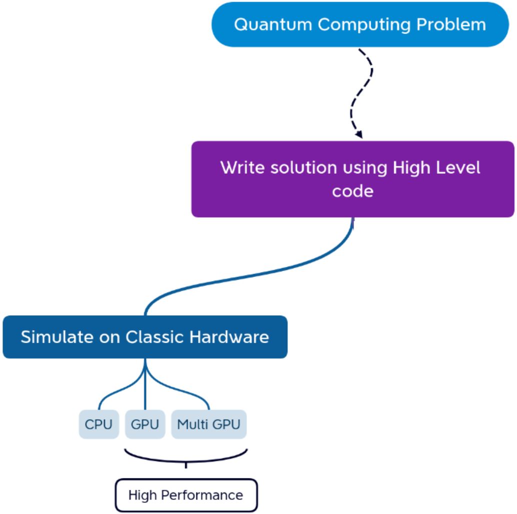
u-quark PDF fit
u f(x)
0.6
0.4
0.2
Approximation
Target u-quark
Ratio
1.025
1.000
0.975
10^-4 10^-3 10^-2 10^-1 10^0
x



Estimates of I_u(Q^2)
I_u(Q^2)
0.230
0.220
0.210
Approximation
Target result
Ratio
1.010
1.000
0.990
0 2500 5000 7500 10000 12500 15000
Q^2 (GeV^2)

Middleware challenges

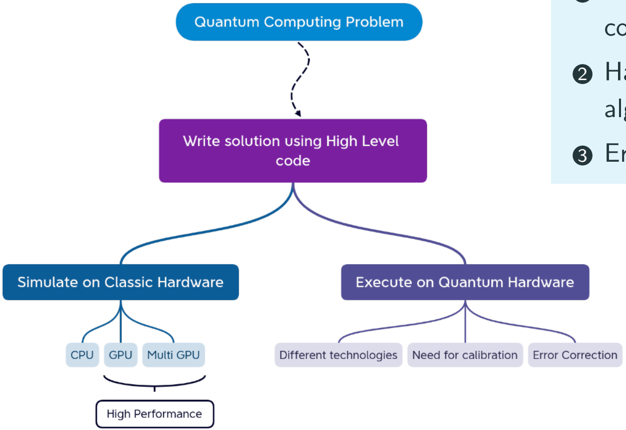
Stage 1: Prototyping models / algorithms



Prototyping

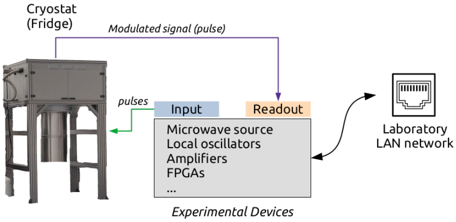
1. High-level quantum circuit programming language
2. Fast classical quantum simulation for model prototyping

Stage 2: Deployment on quantum hardware

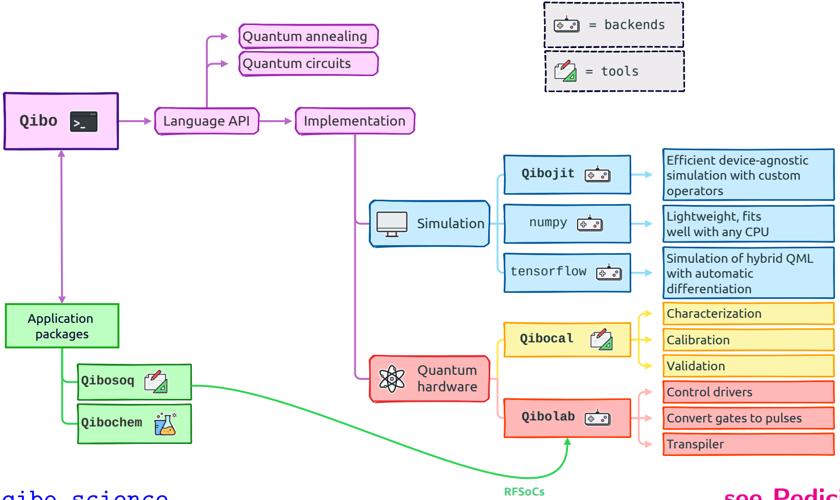


Deployment

1. Gates to microwave pulses sequence compilation (SC qubits)
2. Hardware compatible optimization algorithms
3. Error-mitigation algorithms



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



https://qibo.science

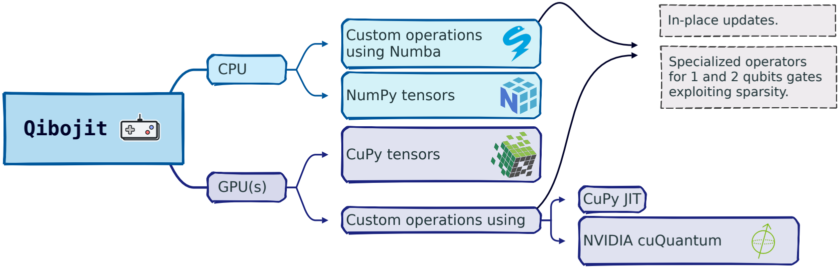
see Pedicillo's talk

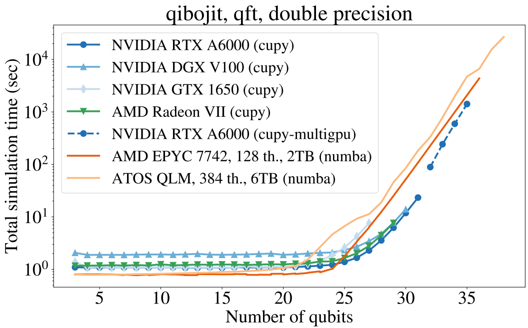
State vector simulation solves:

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

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

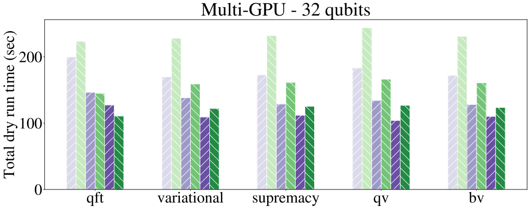
Qibo uses just-in-time technology and hardware acceleration:





Major features:

- Supports CPU, GPU and multi-GPU.
- NVIDIA and AMD GPUs support.
- Reduced memory footprint.

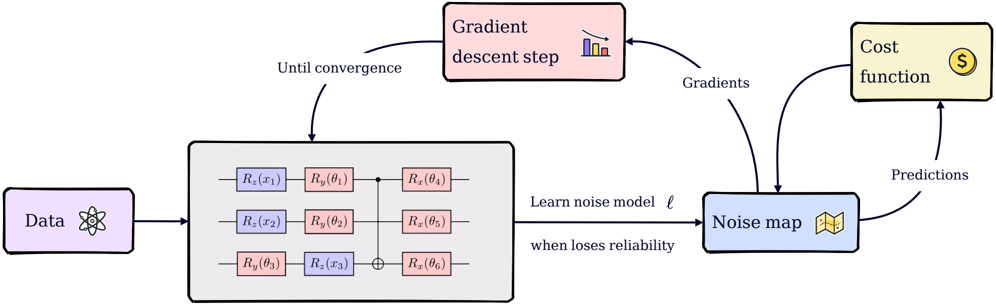


Benchmark library: `https://github.com/qiboteam/qibojit-benchmarks`

see Pasquale's talk

A full-stack example

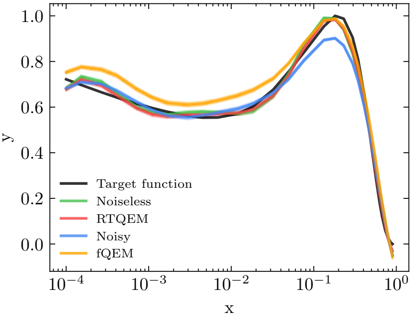
We define a Real-Time Quantum Error Mitigation (RTQEM) procedure.

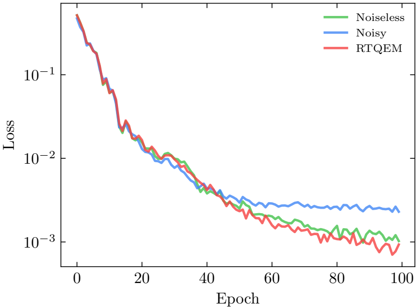


- consider a Variational Quantum Algorithm trained with gradient descent;
- learn the noise map ℓ every time is needed over the procedure;
- use ℓ to clean up both predictions and gradients.

One dimensional HEP target: the u-quark PDF 📖 arXiv:2311.05680

Parameter	N_{train}	N_{params}	N_{shots}	MSE$_{\mathrm{rtqem}}$	MSE$_{\mathrm{nomit}}$	Noise
Value	30	16	10^4	0.008	0.018	local Pauli





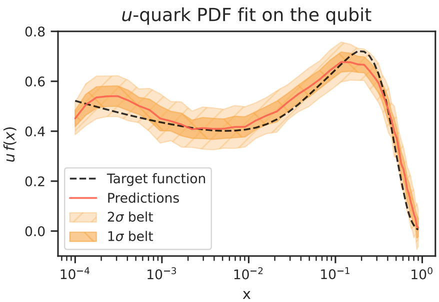
1. thanks to the RTQEM procedure, we reach a good minimum of the cost function;
2. the QEM is not effective is applied to a corrupted scenario (orange curve).

1. High-Level API (Qibo)

- Define model prototype.
- Implement training loop.
- Perform training using simulation.

2. Execution on hardware

- Allocate calibrated platform.
- Compile and transpile circuit.
- Execute model and return results.



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

see Robbiati's talk

Outlook

Outlook

We have observed a great set of interesting **proof-of-concept** applications in HEP.

For the future:

- Improve results quality, moving from **prototype to production**.
- Mitigate hardware noise by implementing **real-time error mitigation** techniques.
- Provide **software tools** for further enhancement of quantum technologies.
- Enhance **calibration, characterization and validation** techniques.
- Codevelop **quantum hardware and instruments** for application specific tasks.