Quantum computing for LHC applications

Stefano Carrazza

June 6th, 2023

PSR2023, UNIMIB

Towards quantum computing

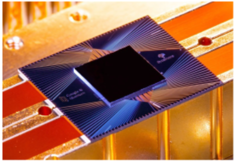
We are moving towards new technologies, in particular hardware accelerators:

CPU

GPU

FPGA/ASIC

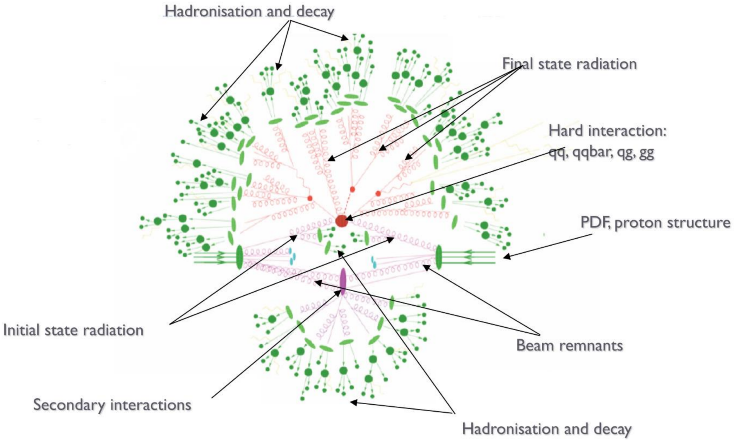
Quantum chip



Moving from general purpose devices $\Rightarrow$ application specific

Physics context: Hadronic collisions at the LHC

Monte Carlo event simulation is **very intensive** and requires lots of **computing power**.



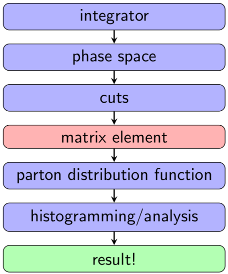
Parton-level Monte Carlo generators

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

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

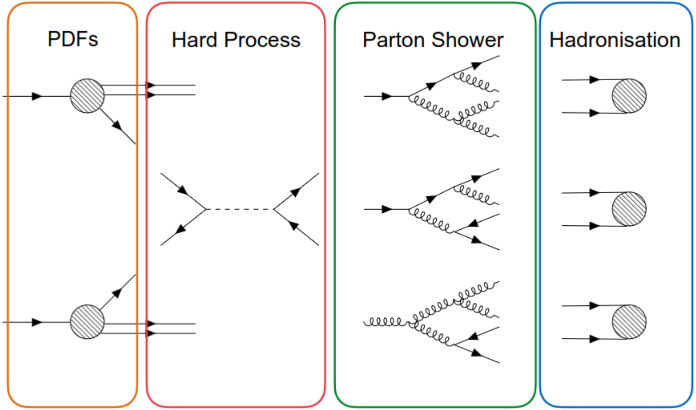
a multi-dimensional integral where:

- $|\mathcal{M}|$ 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.

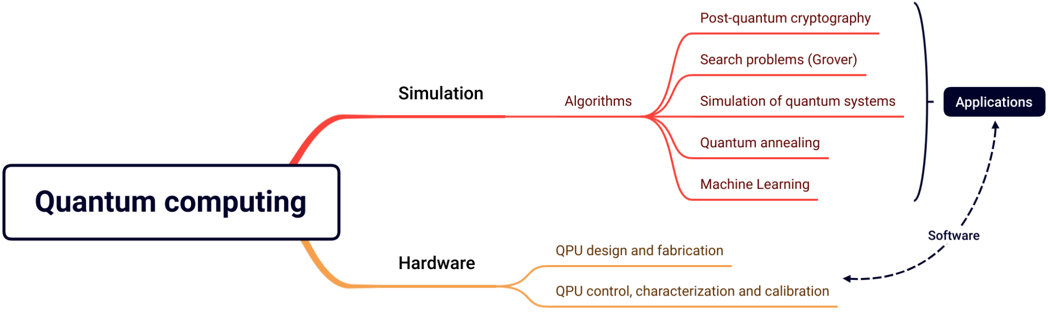


$\Rightarrow$ **Procedure driven by the integration algorithm.**

Monte Carlo generator pipeline

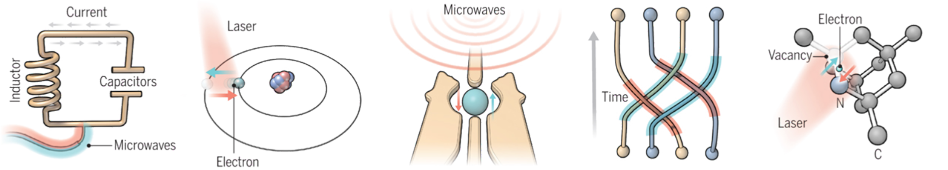


Quantum computing challenges



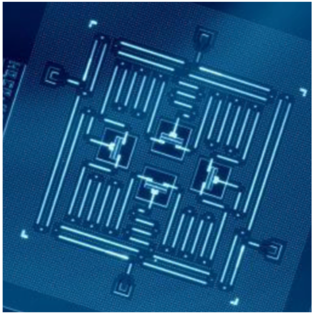
Applications towards quantum advantage must preserve synergy between simulation and hardware.

Quantum Technologies

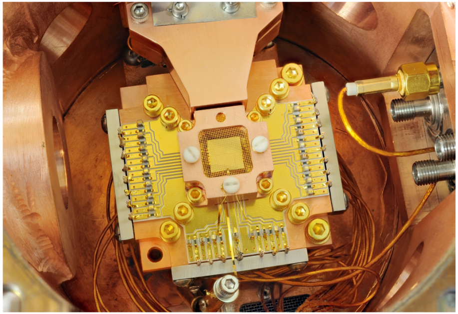


	Superconducting loops	Trapped ions	Silicon quantum dots	Topological qubits	Diamond vacancies
	A resistance-free current oscillates back and forth around a circuit loop. An injected microwave signal excites the current into super-position states.	Electrically charged atoms, or ions, have quantum energies that depend on the location of electrons. Tuned lasers cool and trap the ions, and put them in superposition states.	These "artificial atoms" are made by adding an electron to a small piece of pure silicon. Microwaves control the electron's quantum state.	Quasiparticles can be seen in the behavior of electrons channeled through semi-conductor structures. Their braided paths can encode quantum information.	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.
Number entangled	9	14	2	N/A	6
Company support	Google, IBM, Quantum Circuits	ionQ	Intel	Microsoft, Bell Labs	Quantum Diamond Technologies
Pros	Fast working. Build on existing semiconductor industry.	Very stable. Highest achieved gate fidelities.	Stable. Build on existing semiconductor industry.	Greatly reduce errors.	Can operate at room temperature.
Cons	Collapse easily and must be kept cold.	Slow operation. Many lasers are needed.	Only a few entangled. Must be kept cold.	Existence not yet confirmed.	Difficult to entangle.

Physical implementation



(a) Superconducting device assembled by IBM



(b) Chip based on trapped ions techology

NISQ era

$\Rightarrow$ **We are in a Noisy Intermediate-Scale Quantum era** $\Leftarrow$

(i.e. hardware with few noisy qubits)

How can we contribute?

- Develop new algorithms

  $\Rightarrow$ using classical simulation of quantum algorithms

- Adapt problems and strategies for current hardware

  $\Rightarrow$ hybrid classical-quantum computation

Quantum Algorithms

Some families of algorithms:

Gate Circuits

- Search (Grover)
- QFT (Shor)
- Deutsch
- ...

Variational (AI inspired)

- Eigensolvers
- Autoencoders
- Classifiers
- ...

Annealing

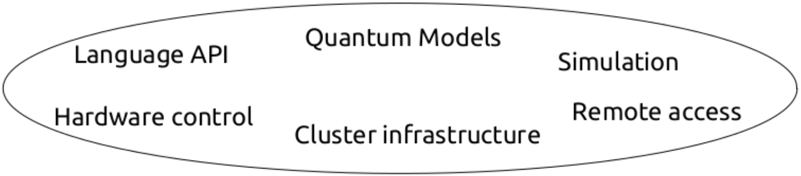
- Direct Annealing
- Adiabatic Evolution
- QAOA
- ...

Quantum software challenges

Challenges

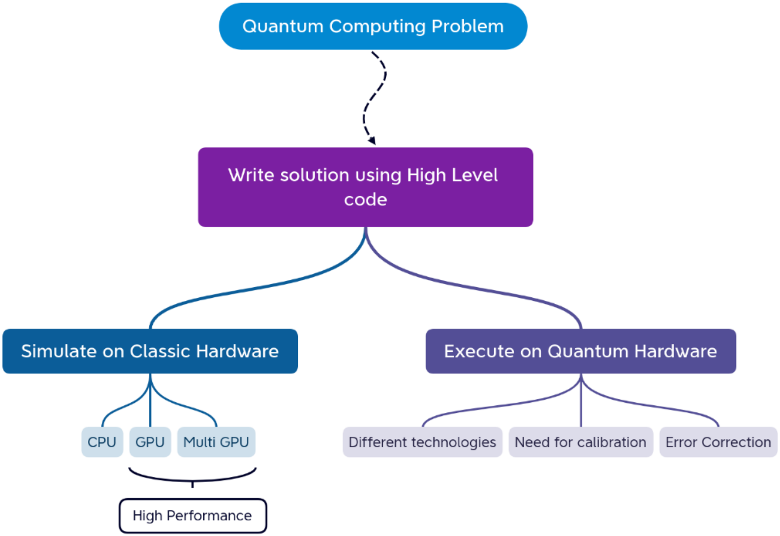
Researcher's needs (lab and theory):

1. Access to **interdisciplinary set of software tools** for:

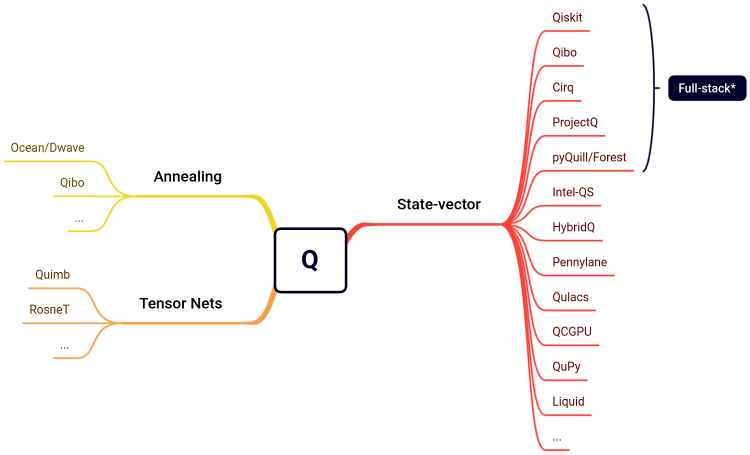


2. **Open-source software** linked to benchmarks and publications.
3. Collaborative development and **definition of standards**.

Challenges


Quantum Computing Problem
Write solution using High Level code
Simulate on Classic Hardware
Execute on Quantum Hardware
CPU
GPU
Multi GPU
High Performance
Different technologies
Need for calibration
Error Correction

Quantum simulation approaches



- Frameworks provide similar features.
- Performance is not always consistent among libraries.

Example: quantum circuit simulation via state-vector

The quantum circuit model considers a sequence of unitary quantum gates:

$$|\psi'\rangle = U_2 U_1 |\psi\rangle \quad \rightarrow \quad |\psi\rangle \text{ — } \boxed{U_1} \text{ — } \boxed{U_2} \text{ — } |\psi'\rangle$$

The final state $|\psi'\rangle$ is given by:

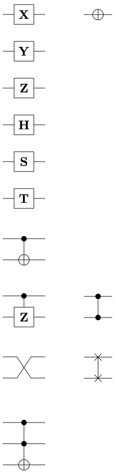
$$\psi'(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\sigma}'} U_1 U_2(\boldsymbol{\sigma}, \boldsymbol{\sigma}') \psi(\sigma_1, \ldots \sigma'_{i_1}, \ldots, \sigma'_{i_{N_{\text{targets}}}}, \ldots, \sigma_N),$$

where the sum runs over qubits targeted by the gate.

- U_2 and U_1 are gate matrices which act on the state vector.
- ψ is a state and it is bounded by memory.

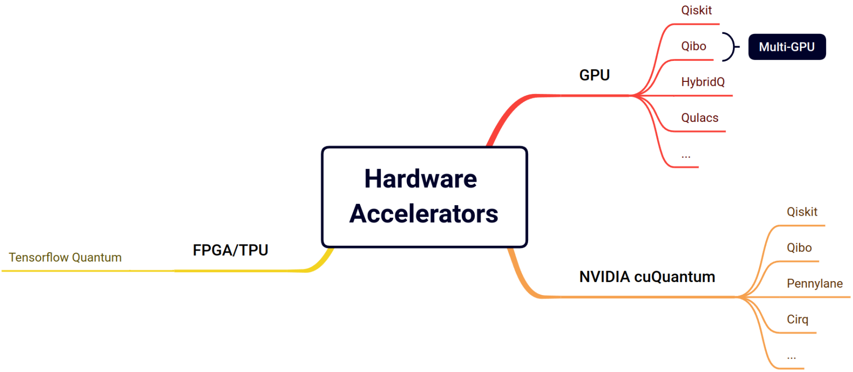
Quantum gates

- **Single-qubit gates**
  - Pauli gates
  - Hadamard gate
  - Phase shift gate
  - Rotation gates
- **Two-qubit gates**
  - Controlled gates
  - Swap gate
  - fSim gate
- **Three-qubit gates**
  - Toffoli



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

Quantum simulation hardware

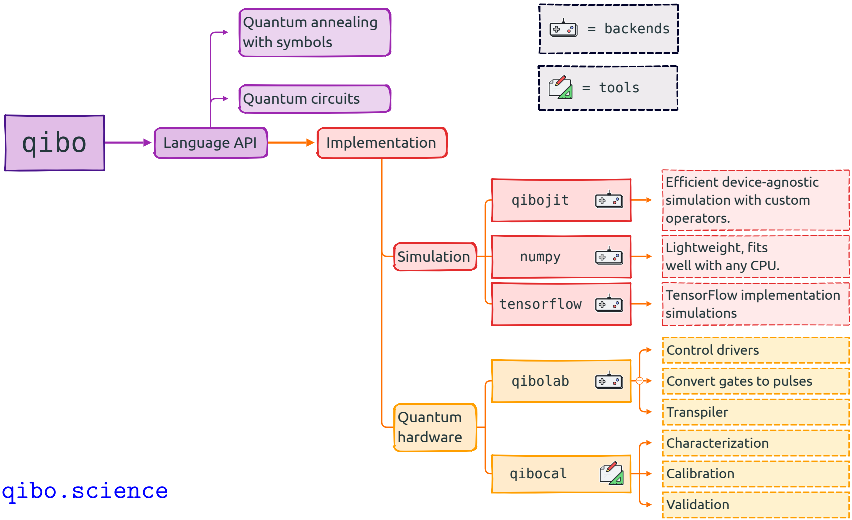


- Frameworks are mostly designed for single-node setups.
- GPUs usage is becoming popular (see cuQuantum SDK).
- Multi-node setups are not simple to deploy.

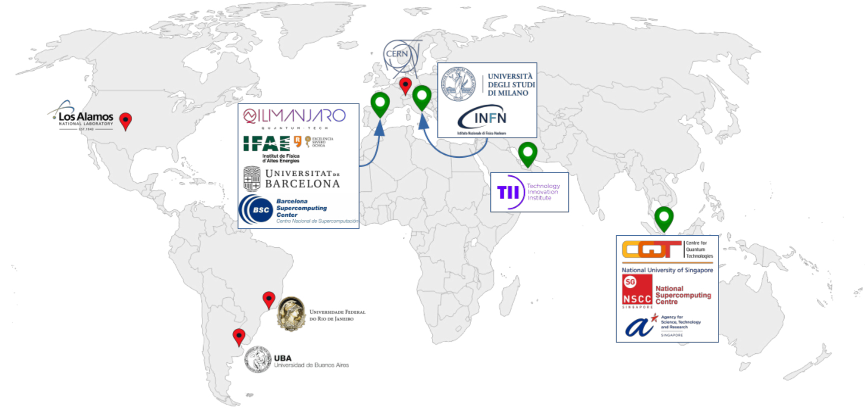
Introducing `Qibo`

Introducing Qibo

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



https://qibo.science



Laboratory	Country	Technology	Qubits
INFN	Italy	Superconducting	1
UNIMIB	Italy	Superconducting	1*
TII	UAE	Superconducting	1, 2, 5, 25
Qilimanjaro	Spain	Superconducting	1 and 2
CQT	Singapore	SC and trapped ion	10

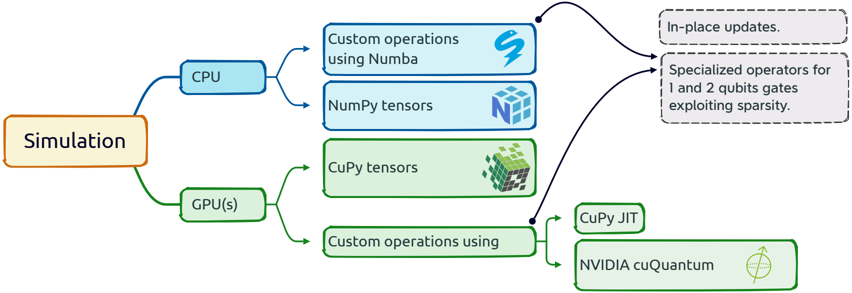
Quantum simulation benchmarks

State vector simulation solves:

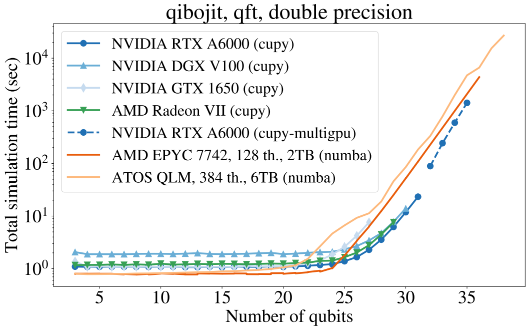
$$\psi'(\sigma_1, \dots, \sigma_n) = \sum_{\boldsymbol{\tau}'} G(\boldsymbol{\tau}, \boldsymbol{\tau}')\psi(\sigma_1, \dots, \boldsymbol{\tau}', \dots, \sigma_n)$$

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

Qibo uses just-in-time technology:

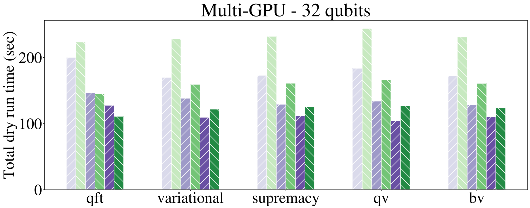


Quantum simulation benchmarks



Major features:

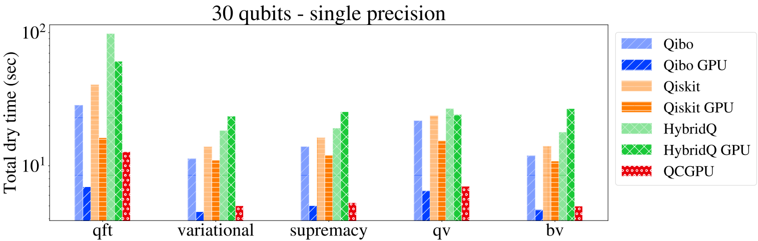
- Supports CPU, GPU and multi-GPU.
- NVIDIA and AMD GPUs support.
- Reduced memory footprint.

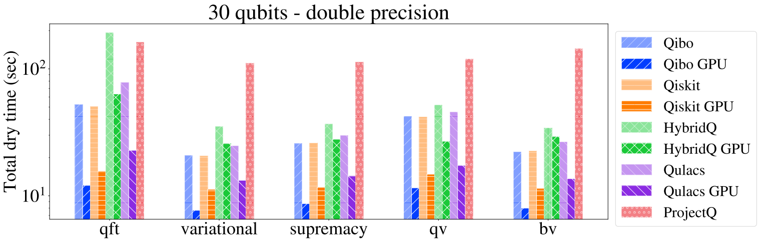


Benchmark library: `https://github.com/qiboteam/qibojit-benchmarks` [arXiv:2203.08826]

Qibo vs other libraries

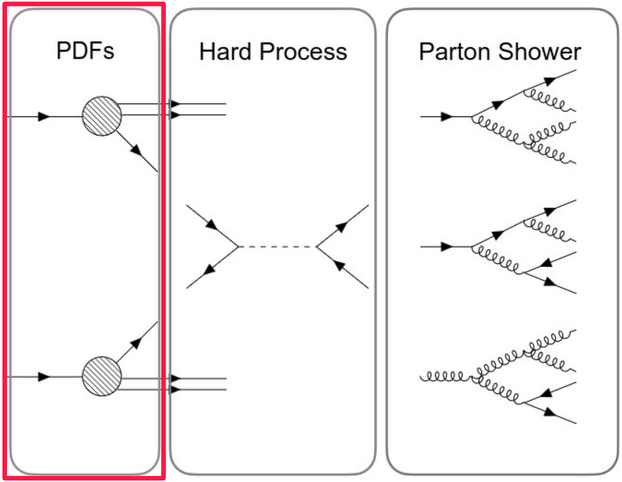
Benchmark library: `https://github.com/qiboteam/qibojit-benchmarks` [arXiv:2203.08826]





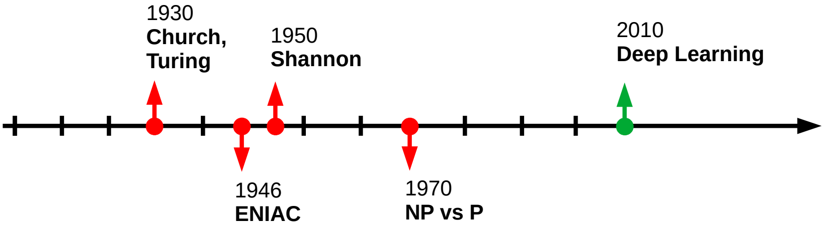
Applications in HEP

The Quantum Disruption

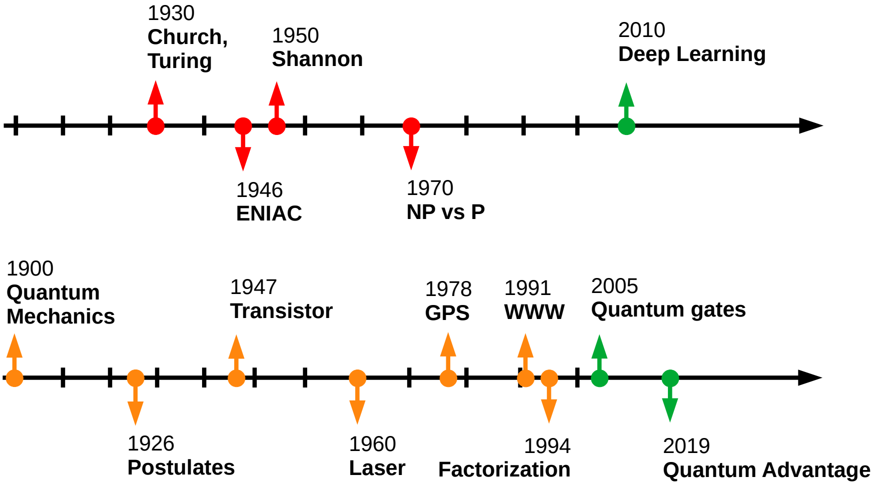


Parton distribution functions
(Machine Learning)

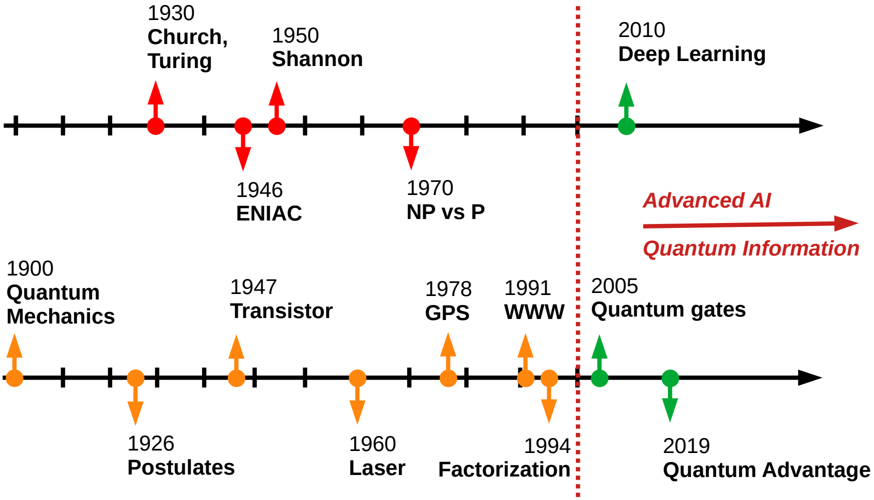
The Quantum Disruption



The Quantum Disruption



The Quantum Disruption

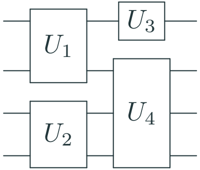


Rational for Variational Quantum Circuits

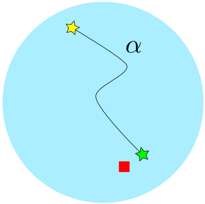
Rational:

Deliver variational quantum states $\rightarrow$ explore a large Hilbert space.

$$U(\vec{\alpha}) = U_n \dots U_2 U_1$$



Near optimal solution

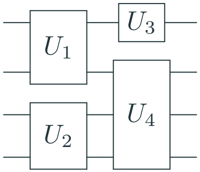


Rational for Variational Quantum Circuits

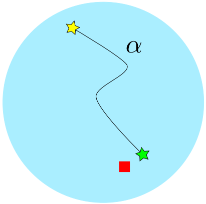
Rational:

Deliver variational quantum states $\rightarrow$ explore a large Hilbert space.

$$U(\vec{\alpha}) = U_n \dots U_2 U_1$$



Near optimal solution



Idea:

Quantum Computer is a machine that generates variational states.

$\Rightarrow$ **Variational Quantum Computer**

Solovay-Kitaev Theorem

Let $\{U_i\}$ be a dense set of unitaries.
Define a circuit approximation to V:

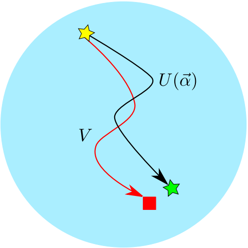
$$|U_k \dots U_2 U_1 - V| < \delta$$

Scaling to best approximation

$$k \sim \mathcal{O}\left(\log^c \frac{1}{\delta}\right)$$

where $c < 4$.

Optimal solution

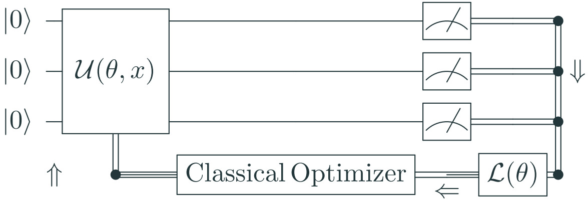


$\Rightarrow$ The approximation is efficient and requires a finite number of gates.

Variational quantum algorithm

How do we parametrize models using a quantum computer?

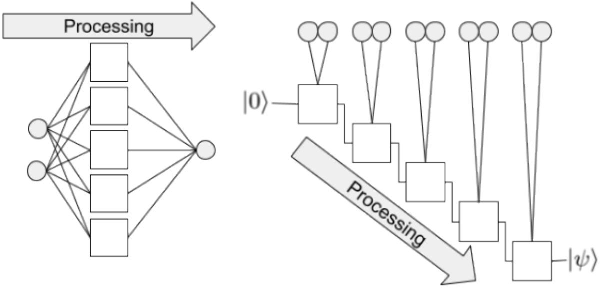
Using variational quantum circuits and data re-uploading algorithms:



Variational quantum algorithm

Pérez-Salinas et al. [arXiv:1907.02085]

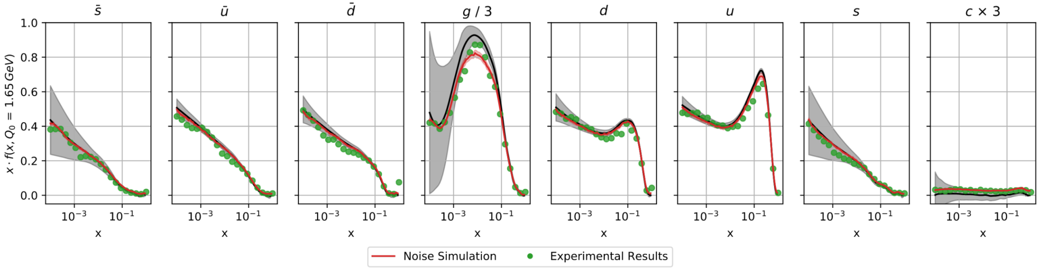
Encode data directly "inside" circuit parameters:

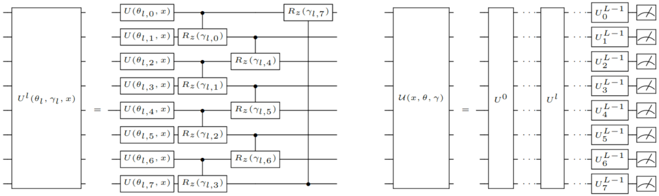


(a) Neural network (b) Quantum classifier

Determination of parton distribution functions using QML

A. Salinas et al, **Determining the proton content with a quantum computer**, PRD, 2011.13934.



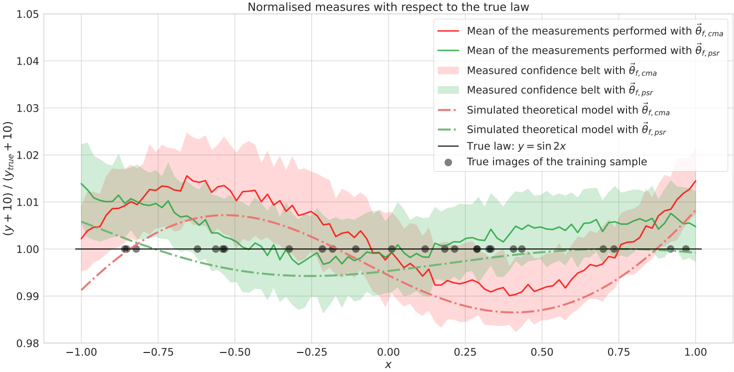


(a) One layer (b) Full Ansatz

Hardware-compatible quantum gradient descent (QGD)

Robbiati et al, 2210.10787.

- Implementation parameter-shift rules to evaluate gradients on hardware
- Results comparable to a genetic optimization.



Error mitigation impact on QGD algorithms

Robbiati et al, 2210.10787.

- Successfully fitting High Energy Physics (HEP) quarks parton density functions in simulation using mitigated-noisy circuits

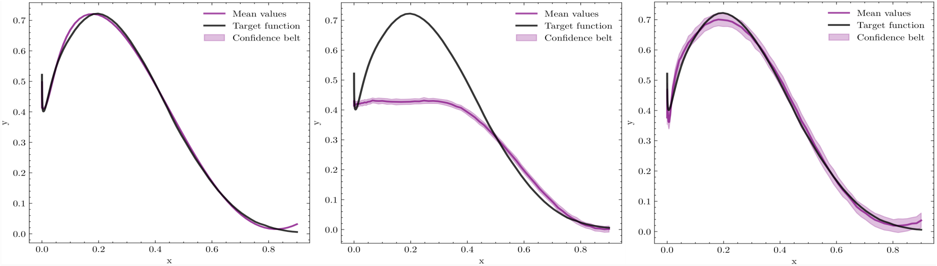
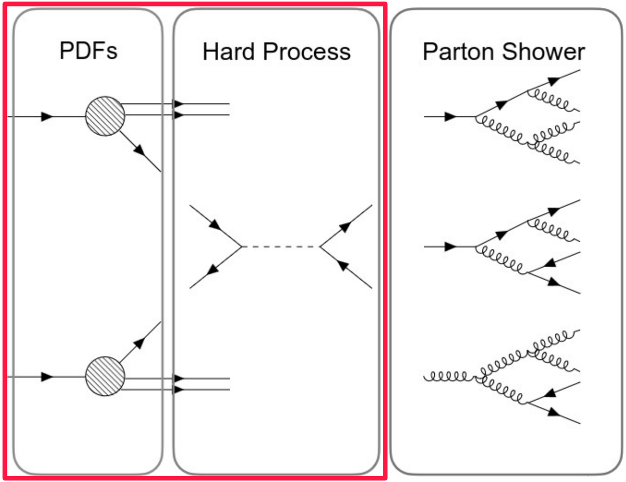


Figure 1: PDF fit performed with different levels of noisy simulation. From left to right, exact simulation, noisy simulation, noisy simulation applying error mitigation to the predictions.

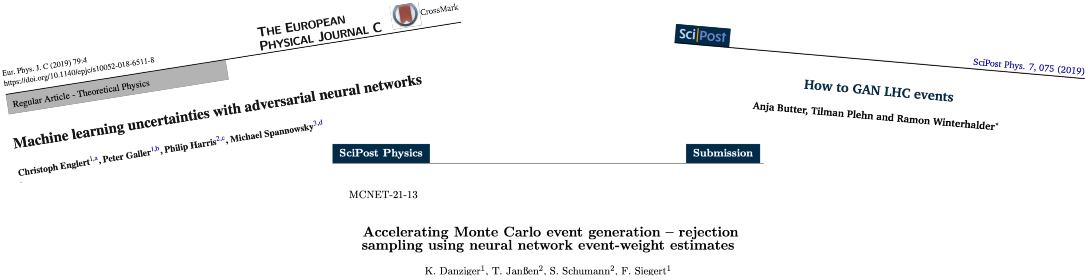
The Quantum Disruption



Event generation

Machine learning approach to event generation

Since 2018, many papers have approached event generation with machine learning techniques:



THE EUROPEAN PHYSICAL JOURNAL C

CrossMark

Eur. Phys. J. C (2019) 79:4
https://doi.org/10.1140/epjc/s10052-018-6511-8

Regular Article - Theoretical Physics

Machine learning uncertainties with adversarial neural networks

Christoph Englert[1,a], Peter Galler[1,b], Philip Harris[2,c], Michael Spannowsky[3,d]

Sci|Post

SciPost Phys. 7, 075 (2019)

How to GAN LHC events

Anja Butter, Tilman Plehn and Ramon Winterhalder*

SciPost Physics | Submission

MCNET-21-13

Accelerating Monte Carlo event generation – rejection sampling using neural network event-weight estimates

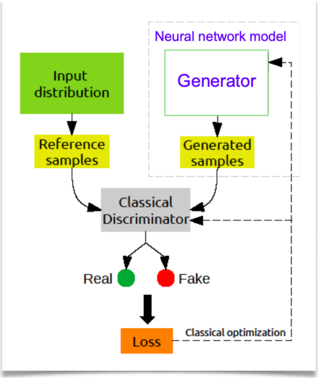
K. Danziger[1], T. Janßen[2], S. Schumann[2], F. Siegert[1]

Main idea ⇒ train with a small dataset, use unsupervised machine learning models to learn the underlying distribution and generate for free a much larger dataset.

Monte Carlo event generation using QGAN

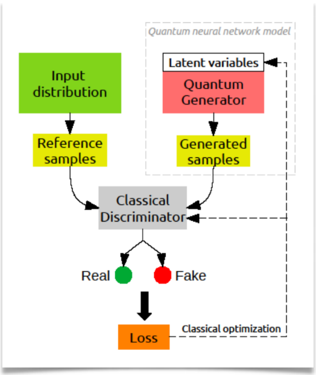
C. Bravo-Prieto et al, 2110.06933

Classical setup:



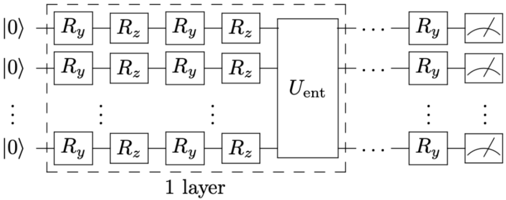
Only the generator becomes quantum

Hybrid quantum-classical setup:



Style-based quantum generator

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**

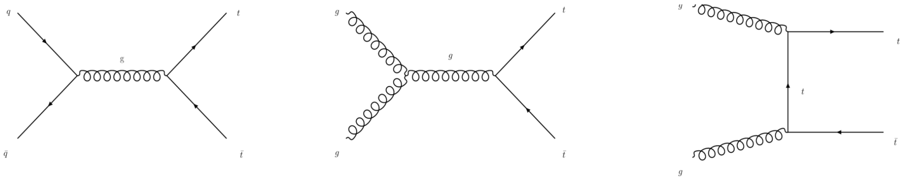
$$R_{y,z}^{l,m}\left(\boldsymbol{\phi_g}, \boldsymbol{z}\right) = R_{y,z}\left(\phi_g^{(l)} z^{(m)} + \phi_g^{(l-1)}\right)$$

Reminiscent of the reuploading scheme

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

Simulation with actual LHC data

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



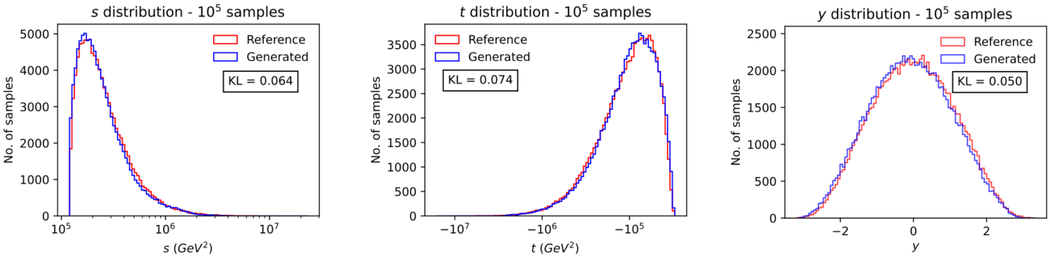
Training and reference samples generated with MadGraph5_aMC@NLO

J. Alwall, et al., JHEP 2014, 79 (2014)

Training set of 10^4 samples, **Mandelstam variables** (s, t) and rapidity y.

Simulation with actual LHC data

After training, we assess the performance with simulations: 3 qubits, 2 layers, 100 bins

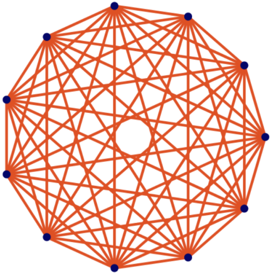


Testing different architectures

Superconducting transmon qubits: *ibmq_santiago* with 2-neighbouring site connectivity

Access via IBM Q cloud service

Trapped ion technology: *ionQ* with all-to-all connectivity



Access via Amazon Web Services

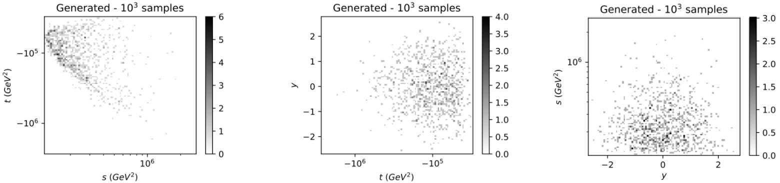
Testing different architectures

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

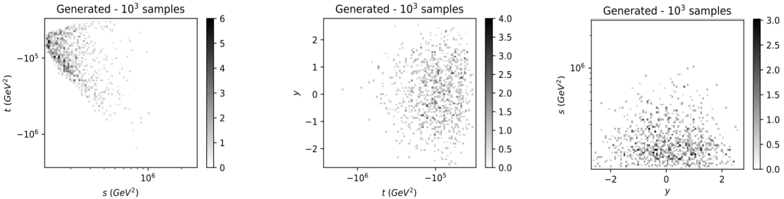
Very similar results:

implementation largely hardware-independent

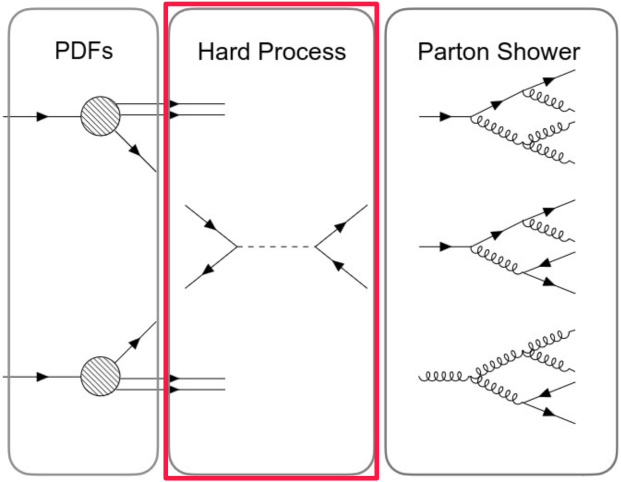
ionQ samples:



IBM Q samples:



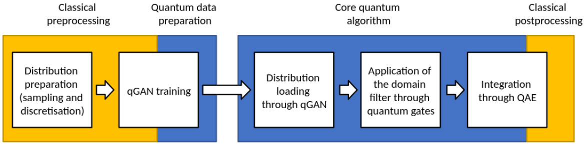
The Quantum Disruption



Monte Carlo Integration

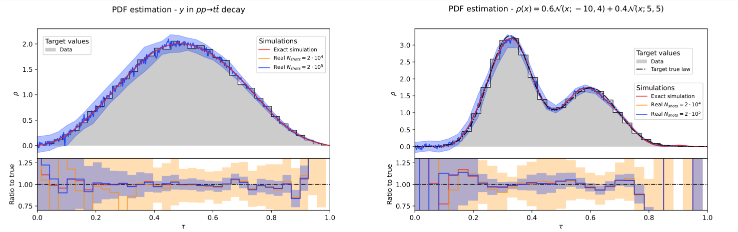
Determining PDFs via adiabatic quantum computing

- Quantum GANs and Quantum Amplitude Estimation for scattering processes.



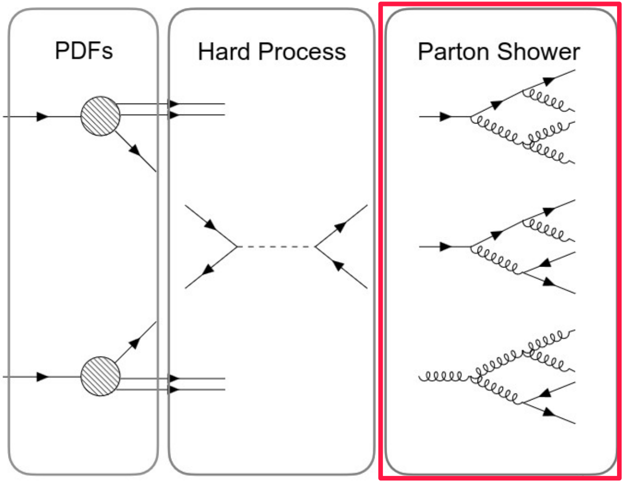
Agliardi et al, 2201.01547.

- Use quantum adiabatic machine learning for the determination of PDF and sampling:



Robbiati et al, 2303.11346.

The Quantum Disruption

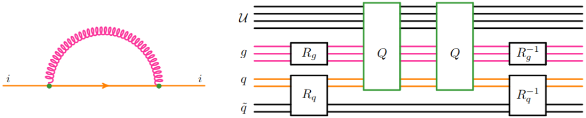


Parton Shower
+Scattering amplitudes

Scattering Amplitudes and Parton Shower

First steps towards generic scattering processes developments:

- Quantum algorithms for Feynman loop integrals — *Ramirez-Uribe et al*, 2105.08703.
- Quantum circuits of colour in perturbative QCD — *Chawdhry et al*, 2303.04818.
- ...

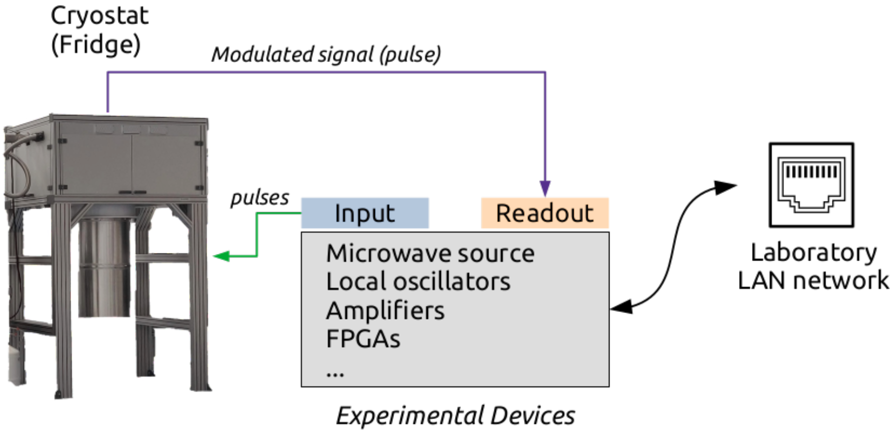


Quantum-based parton shower algorithms:

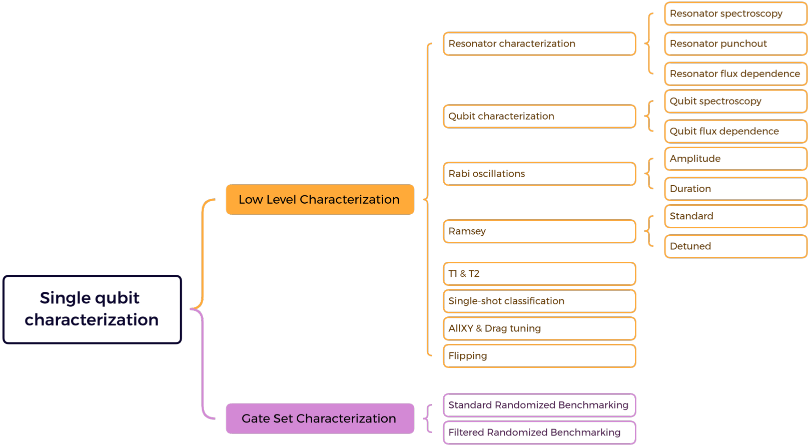
- Polynomial time quantum final state shower — *Bauer et al*, 1903.03196.
- Quantum walk approach — *Bepari et al*, 2109.13975.
- ...

Outlook

Software control challenges



How to characterize and calibrate qubits?



Open-source calibration library: `https://github.com/qiboteam/qibocal` [arXiv:2303.10397]

Outlook

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

- **Phase 1:** reproduce classical results using quantum techniques.
- **Phase 2:** improve the quality of results.

For the future:

- Mitigate hardware noise, implement real-time error mitigation techniques.
- Consider simulations with realistic noise models for hardware emulation.
- Keep in mind that simulation can improve quantum hardware calibration (RB)
- Co-develop quantum hardware design (theory/experiment) for specific applications.