Introducing Qibo

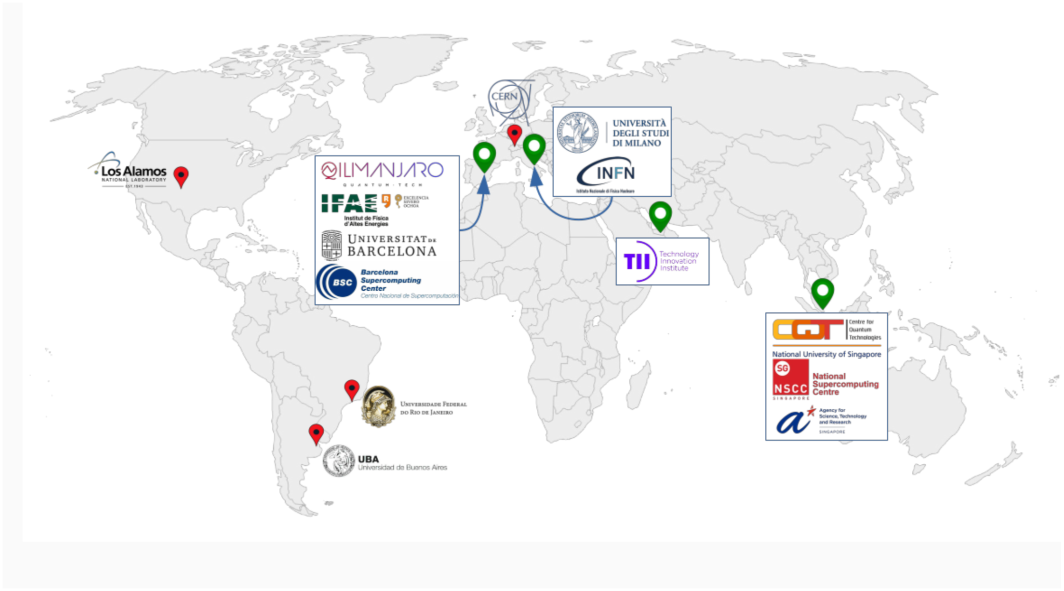
An open-source full stack API for quantum simulation and hardware control

Andrea Pasquale and Stavros Efthymiou on the behalf of the Qibo Team

CINECA Practical Quantum Computing School

Outline of this session

1. Introduction to Qibo
2. Tutorial on how to use Qibo
3. Exercise: Grover's algorithm
4. Your turn to solve the exercise
5. Explanation of the solution
6. Implementation of the solution on GPU


Los Alamos NATIONAL LABORATORY
QILIMANJARO QUANTUM-TECH
IFAE Institut de Física d'Altes Energies
UNIVERSITAT DE BARCELONA
BSC Barcelona Supercomputing Center Centro Nacional de Supercomputación
CERN
UNIVERSITÀ DEGLI STUDI DI MILANO
INFN
TII Technology Innovation Institute
CQT Centre for Quantum Technologies
National University of Singapore
NSCC National Supercomputing Centre Singapore
Agency for Science, Technology and Research Singapore
Universidade Federal do Rio de Janeiro
UBA Universidad de Buenos Aires

Institute	TII	CQT	INFN	Qilimajiaro
Quantum Hardware	5 qubits	10 qubits	1 qubit	2 qubits

Quantum Computing and HPC

Quantum Computing

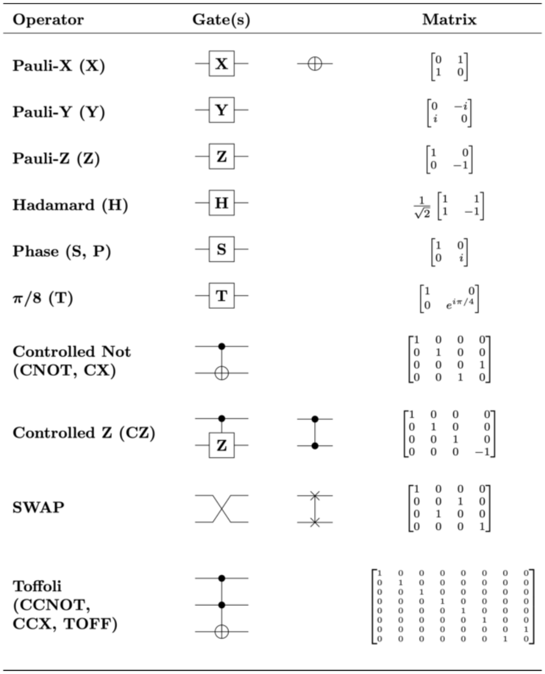
In order to simulate a quantum circuit with n qubits we need to be able to manipulate a 2^n components vector.

In Schrödinger's approach each gate is applied to the state via the following matrix multiplication

$$\psi'(\sigma_1, \ldots, \sigma_n) = \sum_{\boldsymbol{\tau'}} G(\boldsymbol{\tau}, \boldsymbol{\tau'}) \psi(\sigma_1, \ldots, \boldsymbol{\tau'}, \ldots, \sigma_n) \tag{1}$$

where the gate targeting n_{tar} qubits is represented by the $2^{n_{\text{tar}}} \times 2^{n_{\text{tar}}}$ complex matrix $G(\boldsymbol{\tau}, \boldsymbol{\tau'}) = G(\tau_1, \ldots, \tau_{n_{\text{tar}}}, \tau'_1, \ldots, \tau'_{n_{\text{tar}}})$ and $\sigma_i, \tau_i \in \{0, 1\}$.

A few gates



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

- 1 qubit gates 2x2 matrices
- 2 qubit gates 4x4 matrices
- 3 qubit gates 8x8 matrices

Why is it difficult to implement a good quantum simulator?

From the previous slides we can understand that

good **quantum circuits** simulator $\rightleftarrows$ good engine to perform **matrix multiplication**

Moreover, when it comes to full-state vector simulation we need to store to full state vector in the RAM.

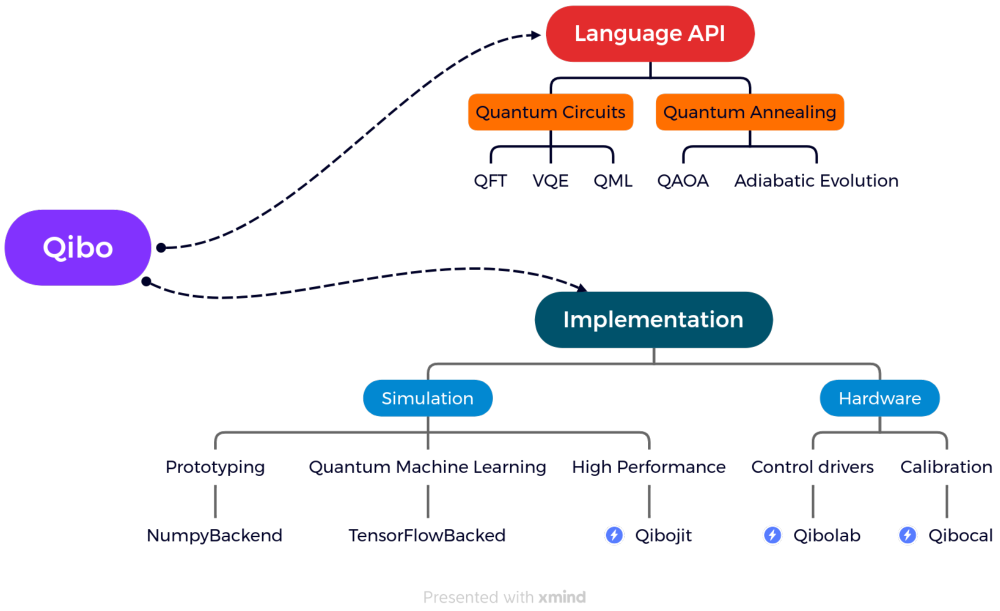
How much memory it is required if we increase the size of the state vector?

Qubits	single precision	double precision
10	8 kB	16 kB
20	8 MB	16 MB
30	8.59 GB	17.18 GB
40	8.79 TB	17.59 TB

Introducing Qibo

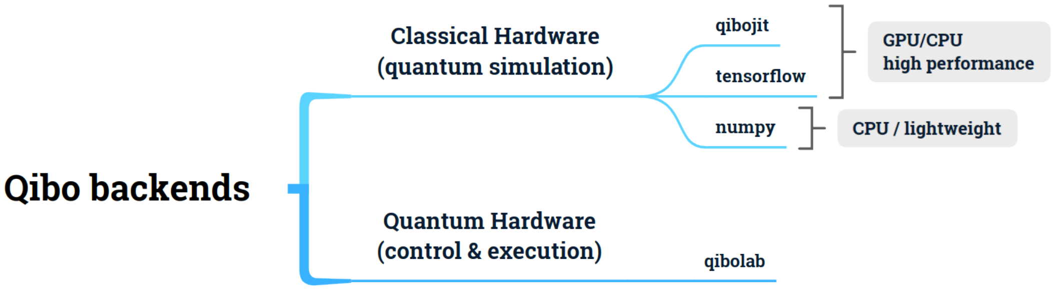
Qibo

Qibo is an **open-source** full stack API for **quantum simulation** and quantum hardware control and calibration.



Simulation backends in Qibo

Qibo provides multiple backends for simulating quantum circuits:



Qibo has a modular layout that enables to switch between different backends easily.

Let's take a closer look at each backend...

Numpy Backend

Simulator based on `numpy`:

- `np.ndarray`
- `numpy` primitives

FEATURES

- Cross-architecture (x86, arm64, etc)
- Cross-platform
- Fast for small circuits
- Fast for single-threaded operations

TensorFlow Backend

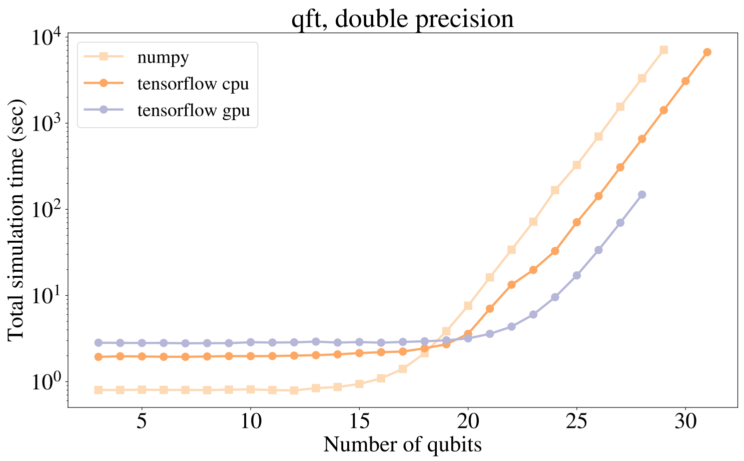
Simulator based on `tensorflow` primitives:

- `tf.Tensor`
- `tf.matmul` and `tf.einsum`

FEATURES

- Multithreading CPU
- Single GPU
- Gradient descent on quantum circuits
- QML using Qibo

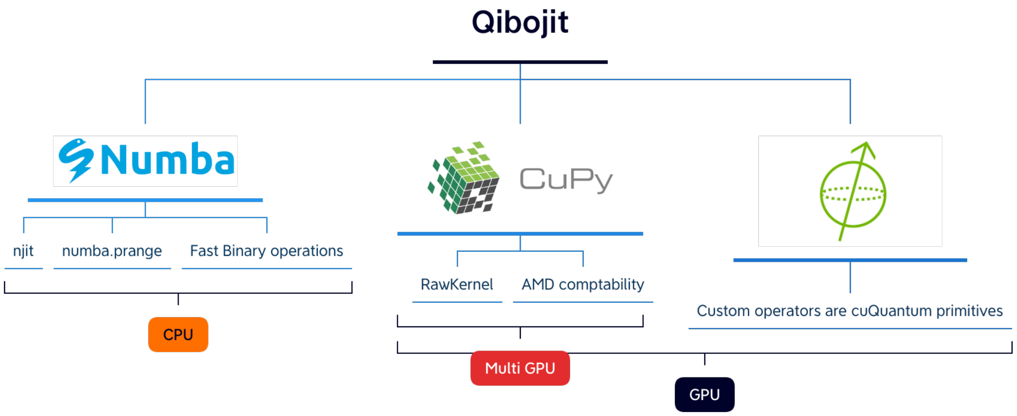
Performance



- Exponential scaling
- Tensorflow better than numpy
- GPU architecture helps with large number of qubits

Can we do better than this?

To efficiently simulate circuits with large number of qubits we designed a new backend in Qibo based on JIT compilation: **qibojit**.



FEATURES

- *in-place* updates
- exploit *sparsity of matrices*
- Just-in-Time compilation
- CuQuantum compatibility

What is Just-in-Time (JIT) compilation?

JIT: a method for improving the performance of interpreted programs.

When compiling/interpreting a language we have different options:

- **Static compiler**: reads a program, looks at the code and tries to convert it into machine code. Examples: C, C++.
- **Interpreter**: looks at the program, does not convert to machine code and it executes it almost as it is. Examples: Python, JavaScript
- **Just-in-Time compiler**: starts a program running an interpreter and dynamically produce machine code based on the observation of the program. Examples: Python, JavaScript

JIT compilers can be **faster** than static compilers because they can get more information by running the program instead of just looking at the program at compile time!

Qibojit - NumbaBackend

```
from numba import njit, prange

@njit(parallel=True, cache=True)
def apply_gate_kernel(state, gate, target):
    """Operator that applies an arbitrary one-qubit gate.

    Args:
        state (np.ndarray): State vector of size (2 **
↪   nqubits,).
        gate (np.ndarray): Gate matrix of size (2, 2).
        target (int): Index of the target qubit.
    """
    k = 1 << target
    # for one target qubit: loop over half states
    nstates = len(states) // 2
    for g in prange(nstates):
        # generate index with fast binary operations
        i1 = ((g >> m) << (m + 1)) + (g & (k - 1))
        i2 = i1 + k
        state[i1], state[i2] = (gate[0, 0] * state[i1] + \
                                gate[0, 1] * state[i2],
                                gate[1, 0] * state[i1] + \
                                gate[1, 1] * state[i2])
    return state
```

Observations

- `@njit`
- `prange`
- fast binary operations

Qibojit - `CupyBackend`

Same approach followed using Numba: JIT compilation.

Custom operators implemented using `cupy.RawKernel`:

1. Write custom CUDA kernels written in C++

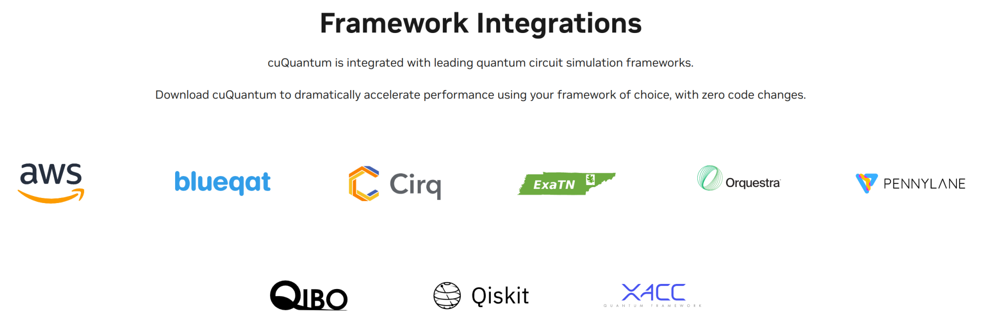
```
apply_gate_kernel = (
    f"""
#include <cupy/complex.cuh>
{_apply_gate}"""
    + """
// C++ implementation of gates.py:apply_gate_kernel()
extern "C"
__global__ void apply_gate_kernel(T* state, long tk, int m, const T* gate) {
  const long g = blockIdx.x * blockDim.x + threadIdx.x;
  const long i = ((long)((long)g >> m) << (m + 1)) + (g & (tk - 1));
  _apply_gate(state[i], state[i + tk], gate);
}
"""
)
```

2. At the first invocation the kernel will be compiled using nvcc
3. After the first invocation it is cached for each device

Qibojit - `cuQuantumBackend`

cuQuantum from NVIDIA has a Python API which delivers all the functionalities `cuStateVec` and `cuTensorNet`.

Thanks to the modular layout of Qibo it was possible to create a new backend where the custom operators are the primitives from `cuStateVec`!



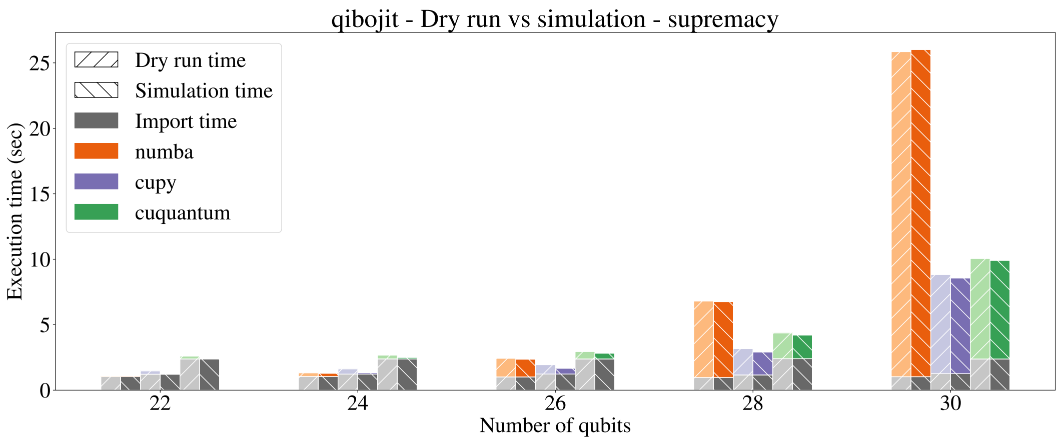
Framework Integrations

cuQuantum is integrated with leading quantum circuit simulation frameworks.

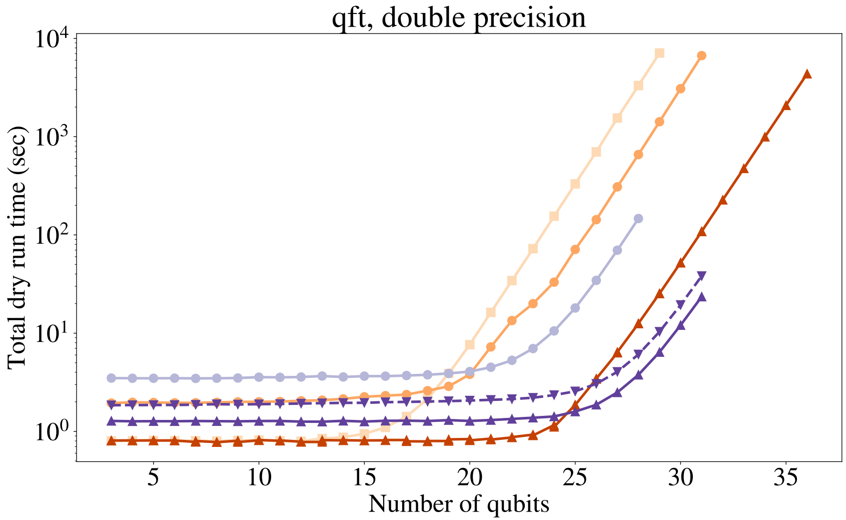
Download cuQuantum to dramatically accelerate performance using your framework of choice, with zero code changes.

Benchmarks

When benchmarking libraries which involve justin-time compilation it is important to distinguish the first execution, *dry run* because it will involve a compilation or loading of cached binaries and therefore will be slower than subsequent executions, *simulation* in the same run time.

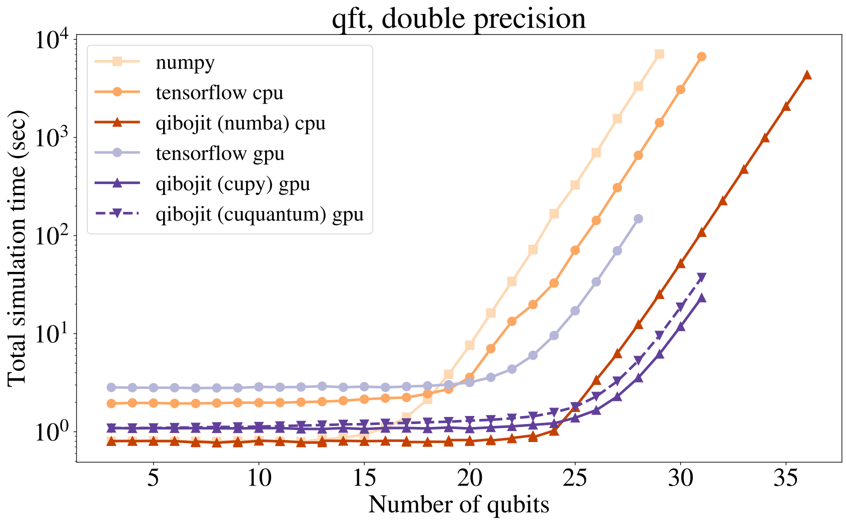


Benchmarks



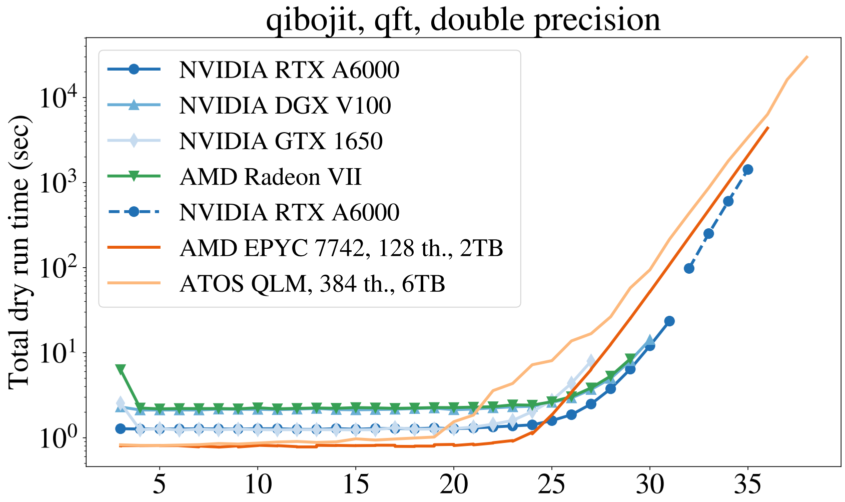
Benchmark library: `https://github.com/qiboteam/qibojit-benchmarks`

Benchmarks



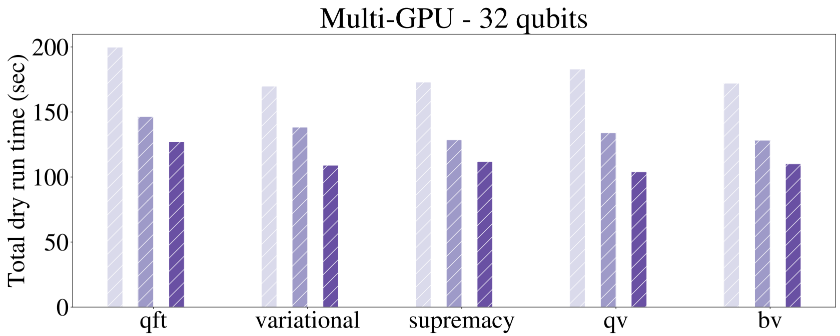
Benchmark library: `https://github.com/qiboteam/qibojit-benchmarks`

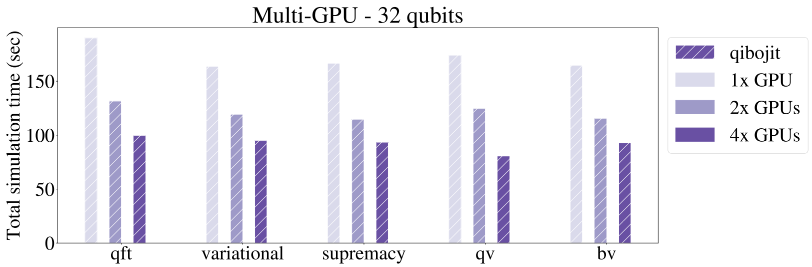
Benchmark on different devices



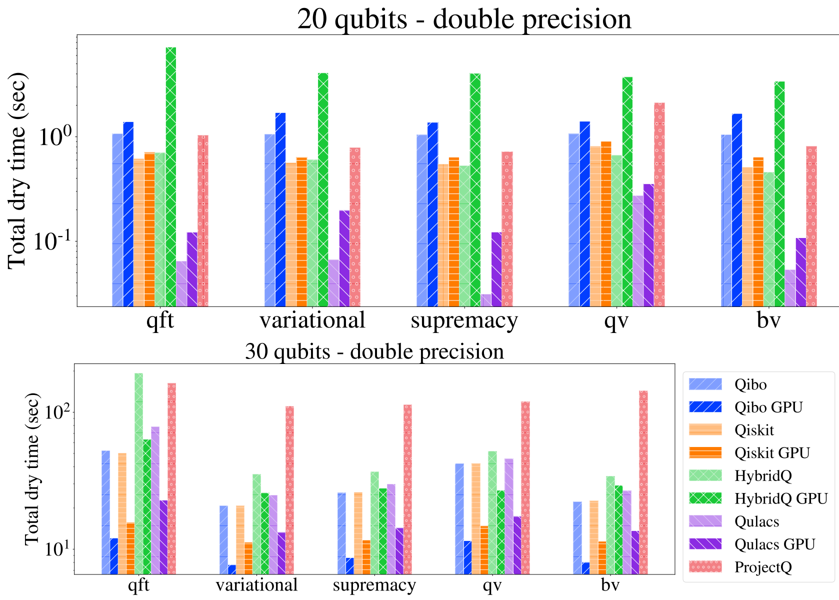
Multi-GPU support

`CupyBackend` supports also multi-GPU architectures





How does Qibo perform against the other libraries?

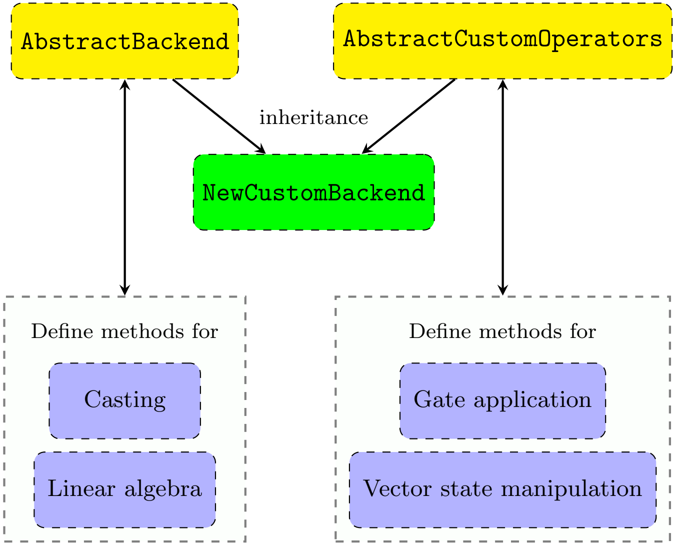


Benchmark library: `https://github.com/qiboteam/qibojit-benchmarks`

How to add a new backend in Qibo?

Do you think that you can develop a backend with better performances?

Thanks to its modular framework in Qibo it is easy to implement a new backend.



Outlook

Outlook

We have presented an open full stack API for quantum simulation: Qibo.

✓ High-performance quantum simulation: **qibojit**

What makes Qibo different from other libraries:

- ✚ Public available as an open source project.
- ✚ Modular layout design with possibility of adding
  - a new backend for simulation
- ✚ Community driven effort

Qibo is **more** than a quantum simulator. We are currently developing modules for

- hardware control $\rightarrow$ `qibolab`
- hardware calibration $\rightarrow$ `qibocal`

`https://github.com/qiboteam/qibo`

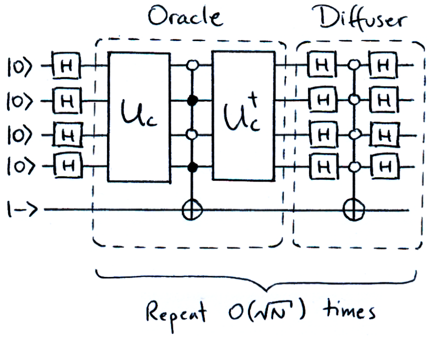
`https://qibo.readthedocs.io/en/stable/`

Thanks for listening!

Grover's algorithm

What is Grover's Algorithm?

Grover's algorithm is a quantum search algorithm that can search for a value or element in an unsorted set in $\mathcal{O}(\sqrt{N})$ as opposed to classical search algorithms that at worse will find an element in $\mathcal{O}(N)$ time.



Quantum advantage originates from:

- **Superposition**: Perform an operation to all possible solutions at the same time.
- **Interference**: Change sign of the amplitude of the correct solution
- **Entanglement**: Non-trivial sharing of information between states

Important operations

Welsh-Hadamard transform: Apply Hadamard gate to every qubit:

$$\mathbf{H} \to \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1 \\ 1 & -1\end{pmatrix}$$

All possible binary strings with equal amplitude amplitude

$$(-1)^{\bar{x}\cdot\bar{y}} 2^{-\frac{n}{2}}$$

Plus or minus sign depending on the number of ones in the initial and final state

Selective face rotation: Apply a phase to just some specific states.

$$\begin{pmatrix} e^{i\phi_{00}} & 0 & 0 & 0 \\ 0 & e^{i\phi_{01}} & 0 & 0 \\ 0 & 0 & e^{i\phi_{10}} & 0 \\ 0 & 0 & 0 & e^{i\phi_{11}} \end{pmatrix}$$

Grover's algorithm uses this matrix with $\phi_i = \pi$ if the state i fulfills a condition, and $\phi_j = 0$ otherwise.

Oracle

Operator that changes the sign of the amplitudes of the quantum states that encode solutions of the problem.

Common way to change the sign once the solution is detected: **use an ancillary qubit**.

Ancilla initialized with an X gate followed by a Hadamard gate:

$$|\psi_a\rangle = HX|0\rangle = H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

When the X gate is applied:

$$X|\psi_a\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |0\rangle) = -|\psi_a\rangle$$

Hint: use CNOT gates to change the sign of the solution.

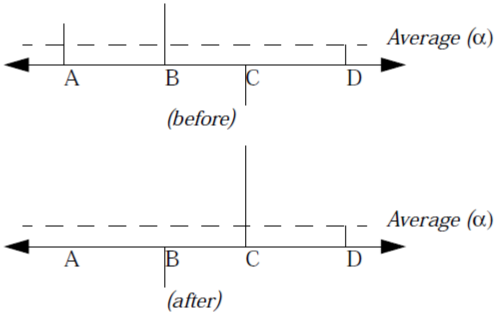
Diffusion transform

The diffusion transform matrix is a matrix defined as follows:

$$D_{ij} = \begin{cases} \frac{2}{N}, & \text{if } i \neq j \\ -1 + \frac{2}{N}, & \text{if } i = j \end{cases} \tag{2}$$

This can be achieved by applying a Welsh-Hadamard transform on all qubits. Then changing the sign of the $|000\ldots000\rangle$ state, and applying once again a Hadamard gate on every qubit.

The diffuser implements an inversion about the average.



Reason for scaling

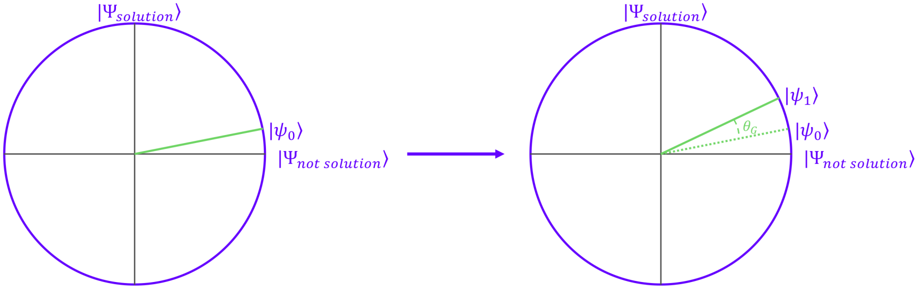
The quantum state can be understood as a superposition of:

$$|\psi_i\rangle = k_i\,|\Psi_{\text{solution}}\rangle + l_i\,|\Psi_{\text{not solution}}\rangle$$

At the start of the algorithm, we can consider $k_0 = \sin\theta$ and $l_0 = \cos\theta$ with $\sin^2\theta = 1/N$.

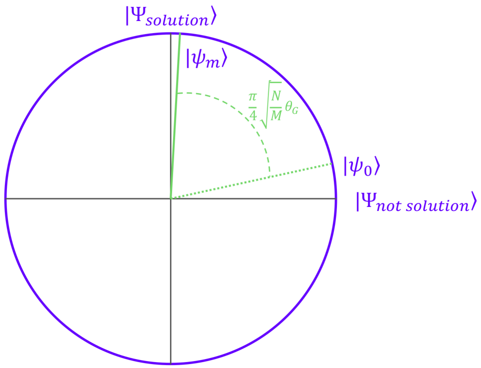
After the i-th Grover step:

$$k_j = \sin(2j+1)\theta \quad \text{and} \quad l_j = \frac{1}{\sqrt{N-1}}\cos(2j+1)\theta$$



$|\Psi_{solution}\rangle$
$|\psi_0\rangle$
$|\Psi_{not\ solution}\rangle$
$|\Psi_{solution}\rangle$
$|\psi_1\rangle$
θ_G
$|\psi_0\rangle$
$|\Psi_{not\ solution}\rangle$

Reason for scaling


$|\Psi_{solution}\rangle$
$|\psi_m\rangle$
$\frac{\pi}{4}\sqrt{\frac{N}{M}}\theta_G$
$|\psi_0\rangle$
$|\Psi_{not\ solution}\rangle$

In order to achieve $k_m = 1$ it follows that
$(2m+1)\theta = \pi/2$
For large number of N:

$$\theta \approx \sin\theta = 1/\sqrt{N}$$

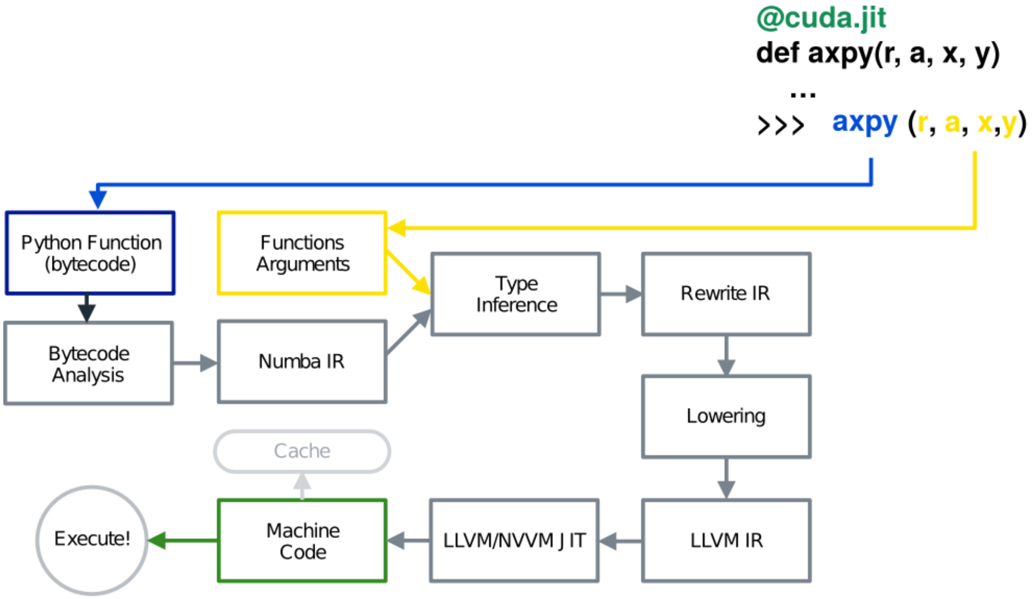
The number of iterations needed is the closest integer to

$$\frac{\pi}{4}\sqrt{N}$$

in case of a single solution.
This can be extended to $\frac{\pi}{4}\sqrt{\frac{N}{M}}$ when considering multiple solutions.

Backup slides

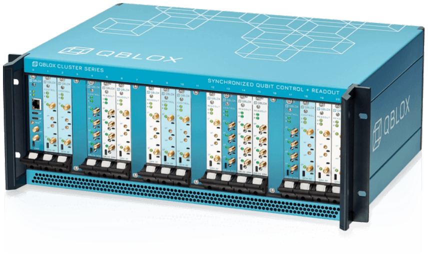
Example of JIT

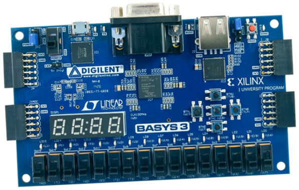


Hardware control using Qibo

Hardware control

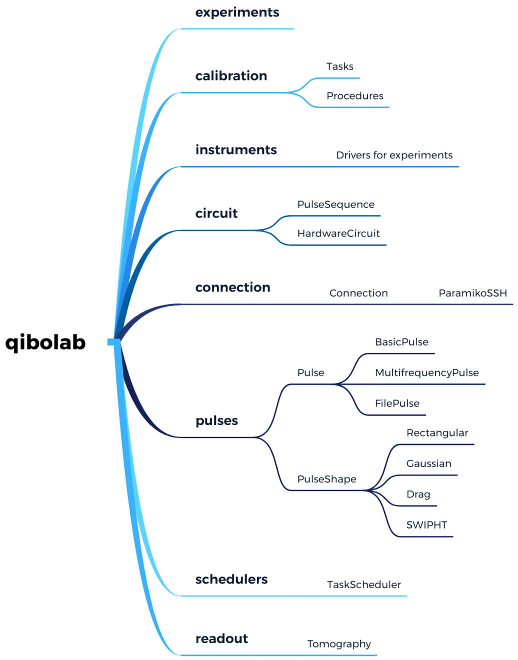
For superconducting qubits **gates** are implemented by sending **pulses**.





We need a framework to control all these devices at the same time.

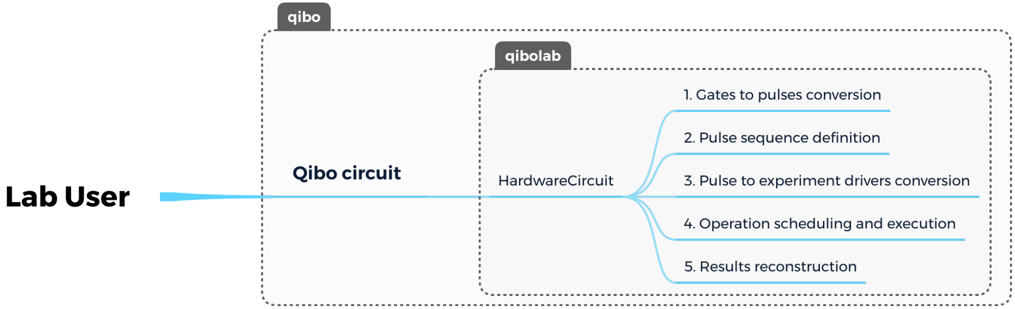
Introducing Qibolab



Qibolab features:

- Deploy Qibo models on quantum hardware easily
- User-friendly Pulse API
- Create custom experimental drivers for lab setup
- Support multiple heterogeneous platforms

How to use qibolab?

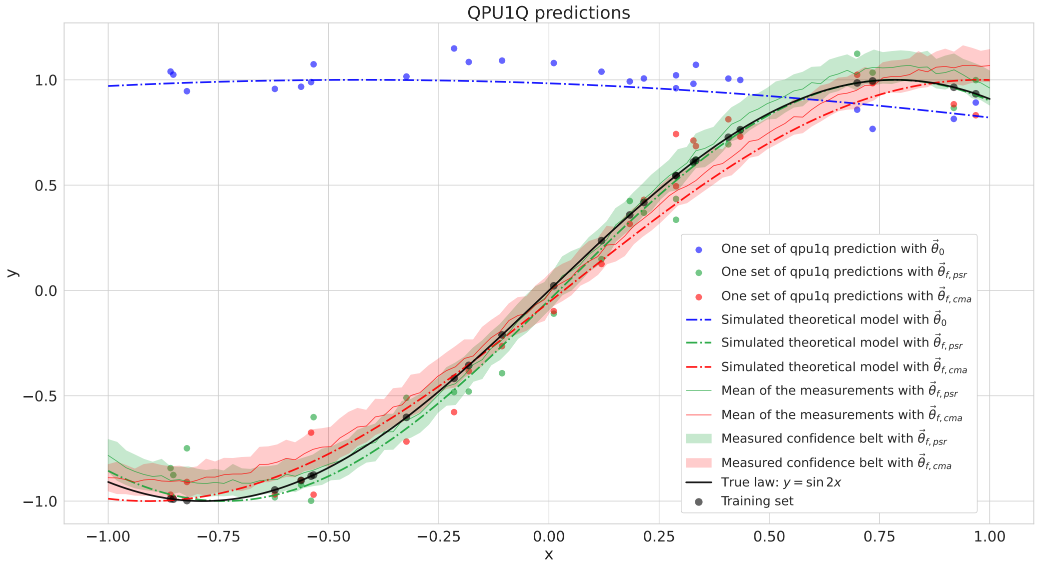

Lab User
qibo
Qibo circuit
qibolab
HardwareCircuit
1. Gates to pulses conversion
2. Pulse sequence definition
3. Pulse to experiment drivers conversion
4. Operation scheduling and execution
5. Results reconstruction

```python
from qibo import models, gates

circuit = models.Circuit(nqubits=1)
circuit.add(gates.H(0))
circuit.add(gates.X(0))
circuit.add(gates.M(0))

# Simulate the circuit
set_backend("qibojit")
simulation = circuit()

# Execute circuit on quantum hardware
set_backend("qibolab")
hardware =  circuit()
```

- A single object to execute both on hardware and simulation
- Job scheduling to access the hardware using slurm

slurm
workload manager

Quantum Machine Learning on Real Hardware



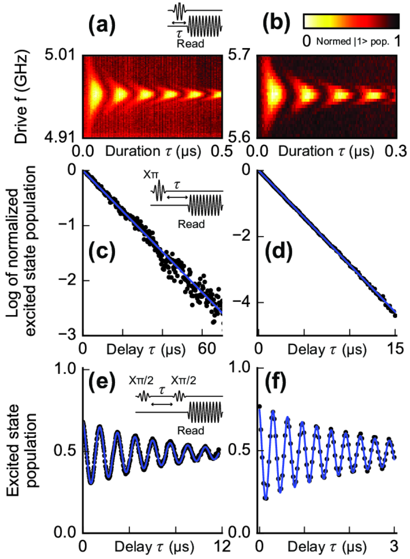
A reporting tool for calibration using Qibo

Difficulties

Suppose that we have assembled a quantum computer and we have a way to send pulses to the chip... are we done? **No**

We need to characterize, validate and verificate our qubits (QCVV):

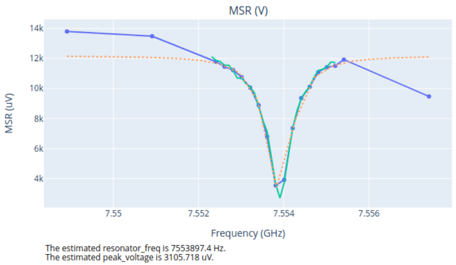
- Perform standard calibration routines:
  - Resonator and qubit spectroscopy
  - Rabi and Ramsey
  - T1 and T2 determination
- Perform quantum protocols to extract the fidelity:
  - Randomized Benchmarking
  - Gate Set Tomography
  - Cross-Entropy Benchmarking
- Repeat the above steps periodically.



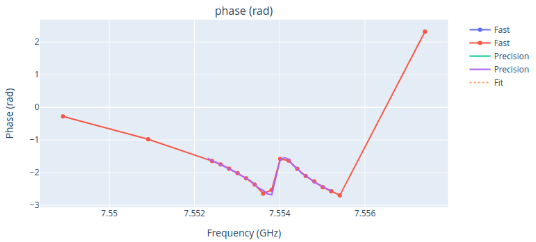
A new reporting tool for Qibo

We are developing a new tool that it will be able to perform QCVV in Qibo with the following features:

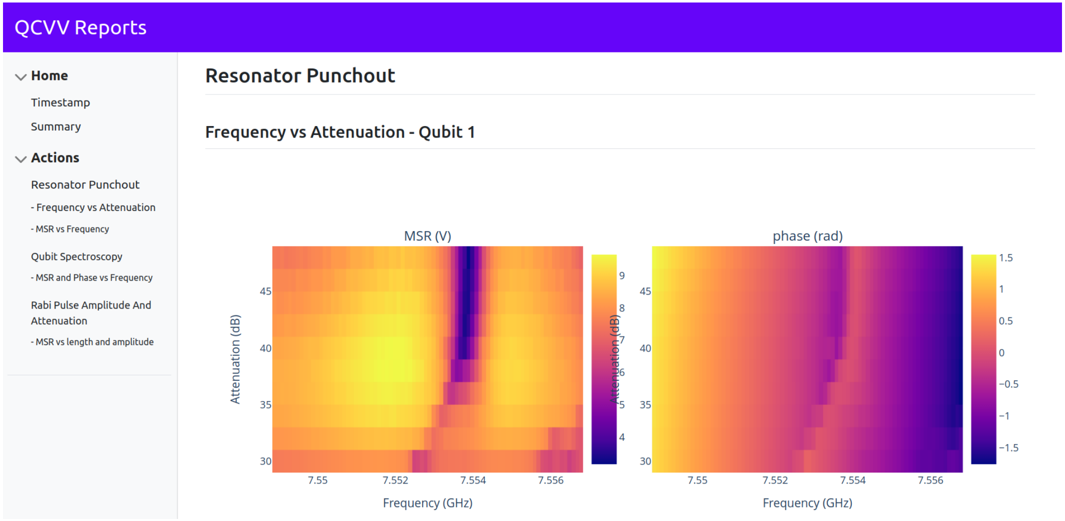
- Platform agnostic
- Launch calibration routine easily
- Live-plotting tools
- Live-fitting tools
- Save and share your data
- Autocalibration routines



The estimated resonator_freq is 7553897.4 Hz.
The estimated peak_voltage is 3105.718 uV.



Report example


QCVV Reports

Home

Timestamp

Summary

Actions

Resonator Punchout

- Frequency vs Attenuation

- MSR vs Frequency

Qubit Spectroscopy

- MSR and Phase vs Frequency

Rabi Pulse Amplitude And Attenuation

- MSR vs length and amplitude

Resonator Punchout

Frequency vs Attenuation - Qubit 1