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Beyond full-state vector simulation with `Qibo`

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Abstract. In this proceedings, we present two new quantum circuit simulation protocols recently added as optional backends to `Qibo`, an open-source framework for quantum simulation, hardware control and calibration. We describe the current status of the framework as for version `0.2.9`. In detail, the two new backends for Clifford and tensor networks simulation are presented and benchmarked against the *state-of-the-art*.

1 Introduction

With the significant achievements reached by quantum technologies [1–3], the interest towards quantum computing is consistently growing. However, the noise affecting these early devices is preventing large-scale applications of quantum algorithms. Waiting for quantum computers to reach a level of reliability that allows for full-scale execution of quantum computing routines without limitations on the problem size, it is necessary to continuously improve the simulation tools we have at our disposal. In particular, the development of classical simulation techniques is crucial to overcome the intrinsic representation limit in full statevector simulation, where the memory required to fully represent a qubit system explodes exponentially as the number of qubits increases.

Several open-source software packages for classical simulation of quantum systems are available. While some of them, including `Qiskit` [4] and `Cirq` [5], `cuQuantum` [6], `tket` [7] and `Yao` [8], provide general tools for quantum simulations, other libraries such as `Pennylane` [9] mostly focus on specific applications like quantum machine learning.

In this context, for the last 4 years we have been developing `Qibo` [10], an open-source software framework for quantum computing. At its early stages, `Qibo` was mainly dedicated to full statevector (including density matrix) simulation [11], and managed to achieve performance competitive with state-of-the-art simulators, thanks, also, to a Just-In-Time compilation approach [12]. The current layout of the `Qibo` framework, as of version `0.2.9`, is shown in Fig. 1. `Qibo` provides a language Application Programming Interface (API) to deploy quantum algorithms using either a circuit-based or a quantum annealing-based approach. Moreover, we provide general-purpose tools that are useful in quantum information theory, including calculation of distances among quantum states and quantum channels. `Qibo`'s modular structure enables the deployment of any component of the language API on different software and hardware platforms, which we refer to as *backends*. We are now going to briefly present all the backends available in version `0.2.9`. The `Qibo` package [13] upon installation is equipped with a backend based on `Numpy` [14], which provides adequate performances for simulating circuits with a relatively low number

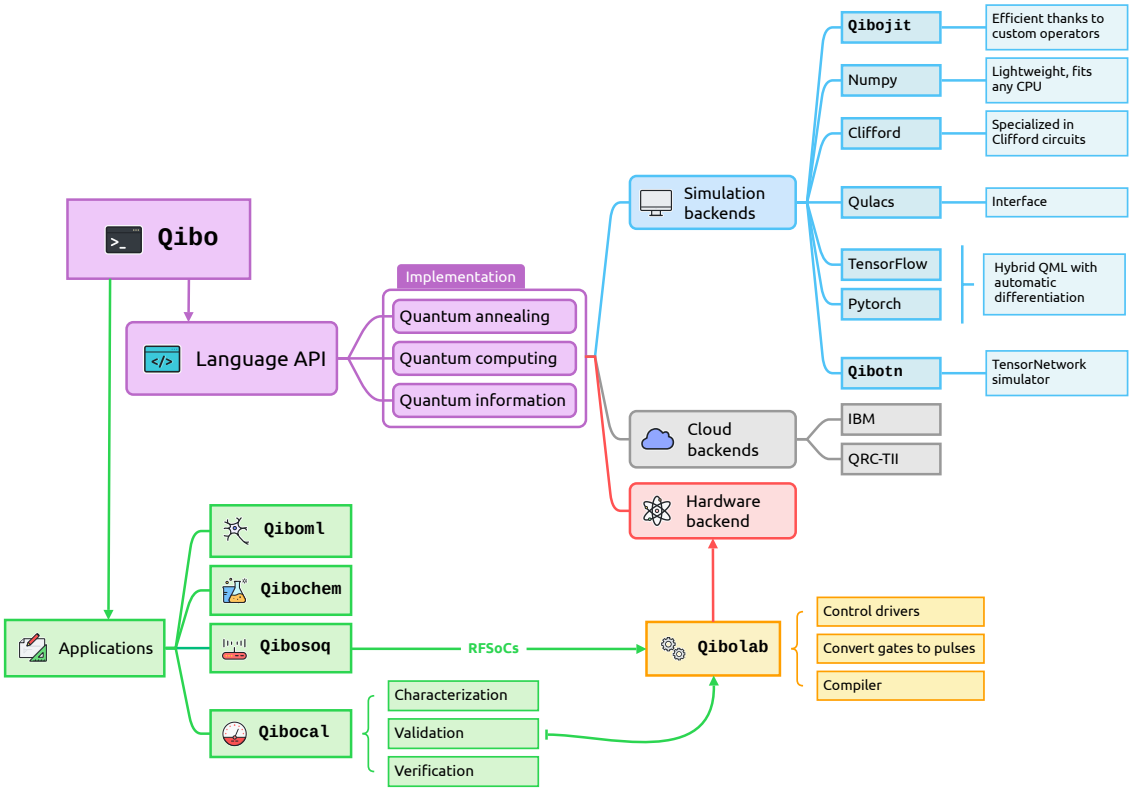


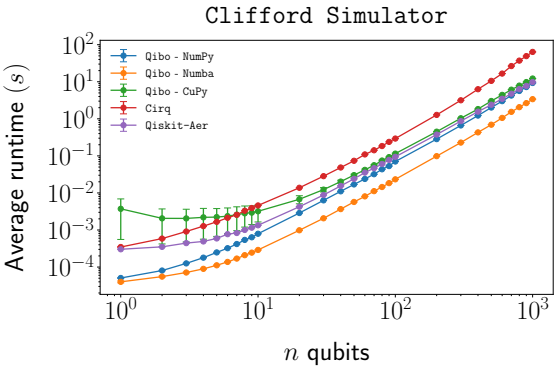
Figure 1: `Qibo` framework in version `0.2.9` [13].

of qubits n (i.e. $n \leq 20$). We also provide a more efficient general purpose simulator, called `Qibojit`, which supports hardware acceleration. More specifically, `Qibojit` allows multi-threaded CPU execution using `Numba` [15], while GPU support is enabled both through `Cupy` [16] and through compatibility with NVIDIA's `CuQuantum` [6] library. To improve the performance, `Qibojit` defines custom operators that exploit the sparsity of the matrix representation of several quantum gates that are often used in quantum computing. Such improvements are also reflected in the quantum annealing approach when the Trotter decomposition is used. We also provide backends supporting automatic differentiation specifically designed for quantum machine learning applications, including one based on `TensorFlow` [17] primitives, and a recently added one based on the popular machine learning framework `Pytorch` [18]. The possibility of integrating automatic differentiation tools within such a modular environment can be exploited to develop and test both pure quantum and hybrid classical-quantum machine learning algorithms [19–25].

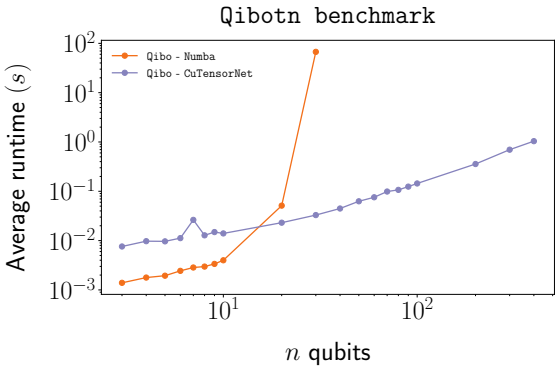
As a middleware software package, `Qibo` also provides a backend for quantum hardware execution. This backend is called `Qibolab`, which defines a dedicated API to perform instrument control, driver operations, as well as compilation of `Qibo` circuits into customizable native gates sets. Alongside `Qibolab`, we provide a dedicated package to characterize and calibrate self-hosted quantum devices: `Qibocal` [26]. Besides simulation and hardware backends, there is an ongoing effort to provide cloud access, giving users the possibility to manage their self-hosted quantum hardware by using `Qibolab`'s hardware control tools, or to deploy quantum circuits on well-known quantum cloud providers, including IBM Quantum [4] and IonQ [27].

This was a brief overview to showcase the wide modularity and diversity that `Qibo` provides. As a demonstration of the ongoing effort to continuously support new platforms and extend `Qibo`'s compatibility with *state-of-the-art* quantum computing software stacks we recently added a backend that interfaces `Qibo` with `Qulacs` [28].

Below, we focus on two simulation backends recently added to the `Qibo` framework, which are dedicated to tensor network simulation of quantum circuits and fast simulation of Clifford circuits.



(a) Simulation of Clifford circuits with an increasing number of qubits. For each point we take the average over 100 different randomly generated circuits. Circuits were generated following Ref. [38], which guarantees an uniform distribution of the generated n-qubit Clifford operators. We did not include measurements in this benchmark.



(b) Total simulation time between `Qibojit` and `Qibotn` for a variational circuit. See [12] for the specific circuit employed. The execution is performed on a `NVIDIA` A100 GPU using NVIDIA and on AMD EPYC 7713.

Figure 2: Benchmarks showing the performances of the Clifford simulator and `Qibotn`.

2 Simulation of Clifford circuits

With full statevector simulation, it is only possible to simulate circuits up to a limited number of qubits: John Preskill describes this limitation in Ref. [29] introducing the approximate yet explanatory term of *50-qubit barrier*. The main limitations are imposed by huge memory requirements and very long computation times [30]. Over the last decades, researchers have studied extensively *Clifford circuits*, a class of circuits that can be simulated in polynomial times [31]. The quantum states generated by Clifford circuits are called *stabilizers states* [32], and have many applications in quantum information theory [33–37]. As current quantum hardware gets closer to the requirements needed for quantum error correction[3], such circuits have started to receive more attention, leading to the development of techniques to classically simulate them.

Based on this, a new backend has been developed in `Qibo` which focuses on fast and efficient simulation of Clifford circuits. The implementation in `Qibo` is based on the phase-space formalism introduced in Ref. [31]. From the perspective of code design, the implementation makes full use of `Qibo`'s modularity, allowing for alternative backends to be easily plugged in. The basic implementation proposed is based on `Numpy` primitives. This enables the single-threaded simulation of Clifford circuits on CPUs. By taking advantage of `Qibojit`, we also provide implementations based on `Numba` and `Cupy`. The integration with the `Numba` backend for multi-threaded computations on CPUs is done via custom kernels that are compiled *just-in-time*. For GPU integration, we make use of custom CUDA C kernels through `Cupy`.

To evaluate our implementation, we compare our Clifford simulator with Clifford simulators available in `Qiskit` and `Cirq`. The results are shown in Fig. 2a. We tested all the simulators on the same dataset consisting of 100 random Clifford circuits for each system syze n. These circuits were sampled uniformly following Ref. [38]. We ran the CPU benchmarks on an AMD EPYC 7773X processor and the GPU benchmarks on a NVIDIA RTX Quadro a6000. Our `Numpy` and `Cupy` backends asymptotically approach performance similar to `Qiskit`, whereas our `Numba`-based implementation displays an advantage over the whole range of qubits considered. For instance, for $n = 1000$, our `Numba` backend is up to one order of magnitude faster than `Qiskit`, and almost two order of magnitudes faster than `Cirq`.

Here, we make a remark about our GPU implementation. As expected, the overhead of copying the data from the host to the device is dominating the results for a small number of qubits. However, an improvement due to the huge parallelization capabilities of GPUs is expected to appear at $n \gtrsim 2^{11}$. Since we benchmarked average runtimes up to 1000 qubits, this "crossing" in performance was not observed yet, making further investigation of bigger systems a necessity.

3 TensorNetwork simulation using `Qibo`

After showing that for specific type of quantum circuits we can reduce the computational time, we now introduce a second popular approach to simulate large quantum circuits: classical approximation

methods. A popular method for approximating quantum circuits are tensor networks (TN) [39], which represents states or operators as network of smaller tensors reducing both memory and computational requirements. They are successfully used, for instance, to solve one-dimensional strongly-correlated quantum systems [40]. On the other hand, the effectiveness of representing large-scale systems comes at the cost of introducing truncation errors, which make these techniques less effective when there is the need to know the quantum state more exhaustively.

Within the `Qibo` framework, we have recently developed `Qibotn`, a `Qibo` subpackage which enables to execute quantum circuits using tensor network like computations, allowing to support large-scale simulation of quantum circuits in `Qibo`. `Qibotn` interfaces `Qibo` with state-of-the-art quantum TN simulation libraries such as `CuTensorNet` [6] from NVIDIA and `quimb` [41]. Both Matrix Product States and generic TN are supported. `Qibotn` is designed to support High Performance Computing configurations including single node GPUs, as well as multi-node multi-GPU configuration using Message Passing Interface or the NVIDIA Collective Communication Library (NCCL) from `NVIDIA`.

To showcase the capabilities of the library we perform comparison between `Qibojit` and `Qibotn` performances in Fig.2b. We execute a variational quantum circuit on a `NVIDIA` A100 GPU for several number of qubits. As expected, using full statevector simulation with `Qibojit` it possible to run only up to 40, while using `Qibotn` we show how the curve flattens and we observe that we are able to simulate a variational circuit with up to 400 qubits. Moreover, given the slow rise of the curve we expect to increase the number of qubits with appropriate memory requirements.

4 Outlook

In this proceedings, we have described the latest updates available in `Qibo 0.2.9`. After a brief overview on all modules currently available in the `Qibo` framework, we have put the focus on two new simulation methodologies: Clifford simulation and Tensor Networks (TN). We have shown that our Clifford simulator is competitive with *state-of-the-art* libraries. We further demonstrated that, despite its early development stage, our TN implementation is able to simulate efficiently circuits with up to 400 qubits. Future developments of the `Qibo` framework include having a dedicated module to perform QML algorithms, which we refer to as `Qiboml`, and we are looking forward to expand `Qibo` to support also quantum chemistry, as well as Quantum optimization problems. Finally, although `Qibo` has been developed in `Python`, we are looking to separate `Qibo` core elements to take advantage of the better performance offered by other languages, e.g. `C++` and `Rust`.

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