MQT Bench: Benchmarking Software and Design Automation Tools for Quantum Computing

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Abstract—Quantum software tools for a wide variety of design tasks on and across different levels of abstraction are crucial in order to eventually realize useful quantum applications. This requires practical and relevant benchmarks for new software tools to be empirically evaluated and compared to the current state of the art. While benchmarks for specific design tasks are commonly available, the demand for an overarching cross-level benchmark suite is not fully met yet and there is no mutual consolidation in how quantum software tools are evaluated thus far. In this work, we propose the *MQT Bench* benchmark suite (as part of the *Munich Quantum Toolkit* (MQT)) based on four core traits: (1) cross-level support for different abstraction levels, (2) accessibility via an easy to use web interface (https://www.cda.cit.tum.de/mqtbench), (3) provision of a broad selection of benchmarks to facilitate generalizability, as well as (4) extendability to future algorithms, gate-sets, and hardware architectures. By comprising more than 30.000 benchmark circuits ranging from 2 up to 130 qubits on four abstraction levels, MQT Bench presents a first step towards benchmarking different abstraction levels with a single benchmark suite.

Index Terms—quantum computing, benchmarking, design automation

I. INTRODUCTION

Quantum computing has gained a lot of attention due to its promising applications and the advances in quantum computing hardware. But currently, designing quantum algorithms often means to manually implement quantum circuits on the gate-level—similar to assembly language in classical computing. Hence, there is an urgent need to enhance the workflow of designing and testing quantum algorithms. Without software tools aiding the design of quantum algorithms, the underlying hardware may not be efficiently utilized. Thus, researchers and developers have already proposed tools for various design tasks, such as quantum circuit simulation [1], [2], compilation [3]–[5], or verification [6]–[10]. This already led to comprehensive quantum circuit design flows realized through toolkits such as IBM's Qiskit [11], Google's Cirq [12], or Rigetti's Forest [13]—in addition to numerous tools and methods developed by other researchers and engineers in the field.

Generally, these software tools operate on and across different levels of abstraction and all tackle computationally hard problems. As a result, they have to compromise between resource demands and result quality. Usually, when a new software tool is proposed, its performance is empirically evaluated. The question how to evaluate the performance of a software tool is very challenging and not yet fully answered—especially for tools solving NP-complete problems. The most common approach is to run certain problem instances, so-called benchmarks, and compare the performance of the newly proposed method against state-of-the-art methods regarding a certain characteristic, e.g., run-time or solution quality.

Currently, this benchmarking is conducted using a wide variety of different benchmark suites—each with a specific focus. While some benchmarks suites, e.g., [14], provide application-oriented benchmarks on a higher abstraction level, other benchmark suites focus on lower abstraction levels, e.g., [15]–[17]. Although the intended target levels are properly covered, the demand for a cross-level benchmark suite is not fully met yet. As another consequence, there is no mutual consolidation which benchmarks to use for empirical evaluations yet—leading to lower comparability, reproducibility, and transparency.

In this paper, we propose *MQT Bench*—another benchmark suite (as discussed above not the first one and most like not the last one) which explicitly aims to address those drawbacks. It aims at providing a first step towards benchmarking the whole quantum software stack with a single benchmark suite by offering the same benchmark algorithms on different levels of abstractions. To realize such a benchmark suite, several challenges have to be tackled:

- Distinct requirements on different levels: Benchmarks have to fulfill certain requirements depending on the abstraction level, e.g., only gates of a device's native gate-set are allowed.
- Accessibility: To foster adoption of the benchmark suite, it needs to be as easy to use as possible.
- Generalizability: Providing a comprehensive set of benchmark algorithms to cover as many use cases as possible.
- Extendability: Future algorithms, gate-sets, and architectures should be easy to integrate.

MQT Bench has been developed with these challenges in mind and is based on four core traits:

1) Cross-level benchmarking: Provision of benchmarks on four abstraction levels.
2) Accessibility: To simplify the usage of MQT Bench, we provide a web interface (https://www.cda.cit.tum.de/mqtbench) in addition to the open-source repository on GitHub (https://github.com/cda-tum/MQTBench).
3) Algorithm selection: Broad selection of different algorithms ranging from building blocks, i.e., *Quantum Fourier Transform* (QFT), to applications, i.e., ground state estimation.
4) Extendability: Algorithms, gate-sets, and hardware architectures are easily extendable and integrable into MQT Bench.

By this, MQT Bench aims to improve the comparability, reproducibility, and transparency of empirical evaluations for the whole quantum software stack.

The rest of this work is structured as follows: In Section II, we review the necessary basics of the quantum computing compilation flow and the respective software stack to keep this work self-contained. Afterwards, Section III reviews the state of the art on how this quantum software stack is currently evaluated and benchmarked—motivating the benchmark suite proposed in this paper. Based on that, Section IV introduces the resulting benchmark suite and its core traits, before Section V concludes this work.

II. BACKGROUND

To keep this paper self contained, this section gives a brief overview of the quantum circuit compilation flow with its different abstraction levels and the respective quantum software stack. The levels mentioned in this section are inspired by the structure proposed by the openQASM 3.0 specification [18] and can similarly be found in many other compilation flows as well.

A. Quantum Circuit Compilation Flow

Similar to the classical domain, executing a conceptual quantum algorithm on an actual device requires compiling it to a representation that adheres to all constraints imposed by the hardware. Usually, quantum algorithms are initially developed and tested at a hardware-agnostic level. Generally, this is described as a quantum circuit that consists of high-level building blocks without any restrictions to a certain gate-set or hardware architecture and is defined as the *algorithmic level*.

Example 1. Variational Quantum Algorithms *(VQAs) are an emerging class of quantum algorithms with a wide range of applications. A respective circuit is depicted in Fig. 1a and shows an example of an ansatz function frequently used for* Variational Quantum Eigensolvers *(VQEs), a subclass of VQAs. On this abstraction level, the circuit is parameterized by the angles θ_i of the six single-qubit gates.*

(a) Algorithmic level   (b) Target-independent level

(c) Target-dependent native gates level   (d) Target architecture: IBMQ Manila
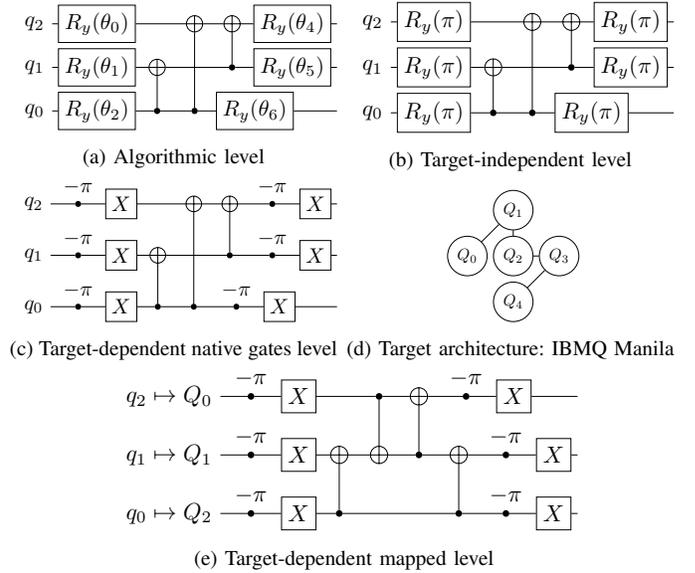

(e) Target-dependent mapped level

Fig. 1. Compilation of a Variational Quantum Algorithm.

The first step in realizing a conceptual quantum algorithm on the algorithmic level for a particular problem is to synthesize the high-level building blocks and optimize the resulting representation independent from an actual target architecture. In analogy to a classical compiler, this involves tasks such as constant propagation and folding, gate modifier evaluation, synthesis, loop unrolling, and gate simplification. The resulting representation is defined as the *target-independent level*.

Example 2. *VQAs are hybrid quantum-classical algorithms, where the parameters of the quantum ansatz are iteratively updated by a classical optimizer analogous to conventional gradient-based optimization. Consider again the circuit from Fig. 1a. Assuming these parameters have been determined, e.g., $\theta_i = -\pi$ for $i = 0, ..., 5$, they are now propagated and the resulting quantum circuit is shown in Fig. 1b.*

Today's quantum devices impose several constraints on the circuits that may be executed on them. Thus, a target-dependent compilation phase is necessary. For one, devices only provide a particular set of native gates—typically consisting of an entangling gate (like the CX gate) and some family of single-qubit gates. Hence, the gates of a circuit need to be translated to this native gate-set, which is typically followed by an optimization pass that aims to reduce the introduced overhead. This representation level is defined as the *target-dependent native gates level*.

Example 3. *Different quantum computer realizations support different native gate-sets. In our example, we consider the IBMQ Manila device as the target device which natively supports I, X, $\sqrt{X}$, R_z, and CX gates. Consequently, the R_y gates in Fig. 1b have to be converted using only these native gates. In this case, they are substituted by a sequence of X and R_z gates (denoted as $\bullet$ with a phase of $-\pi$) as shown in Fig. 1c.*

In addition to the limited gate-set, today's devices (at least those based on superconducting qubits) only feature a limited connectivity between their qubits. Consequently, the circuit's logical qubits need to be *mapped* to the targeted device's physical qubits, so that multiple-qubit gates are only applied to qubits directly connected on the device. Since such a mapping can rarely be determined in a static fashion, i.e., globally for the whole circuit, the mapping has to change dynamically throughout the circuit, which is frequently referred to as mapping or routing. Again, this is followed by a round of optimization in order to minimize the overhead caused by the compilation. This representation level is defined as the *target-dependent mapped level*.

Example 4. *Consider again the scenario from Example 3. The architecture of the IBMQ Manila device is shown in Fig. 1d and it defines between which qubits a two-qubit operation may be performed. Since the circuit shown in Fig. 1c contains CX gates operating between all combination of qubits, there is no mapping directly matching the target architecture's layout. As a consequence, a non-trivial mapping followed by a round of optimization leads to the resulting circuit shown in Fig. 1e. This is also the reason for the different sequence of CX gates compared to the previous example.*

At this point, the circuit is ready to be sent to the quantum computer's backend for execution. From there, the individual gates are scheduled, linked to a particular calibration, and the resulting circuit is eventually passed to the target machine code generator. The resulting binaries are then forwarded to the execution engine to orchestrate the quantum computation on the actual device.

B. Quantum Software Stack

Quantum software is needed on all levels reviewed above in order to aid designers in eventually realizing useful quantum applications. In the following, we review three of the core design tasks for software tools.

As of today, quantum computers are a scarce resource with limited availability and capability. Until more devices become available which are larger and less prone to errors, classical means to simulate quantum algorithm circuits (also known as *quantum circuit simulators*) are essential for fostering the development of quantum applications. Additionally, and in contrast to actual quantum computing devices, quantum circuit simulators allow for detailed insights into the quantum states throughout the circuit execution since the state's amplitudes are explicitly tracked during the simulation. On actual hardware, information can only be extracted in the form of measurements from the final quantum state, which each yields a classical bit string according to the distribution described by the state's amplitudes. Such simulators can be used on the highest possible level of abstraction, since they can be designed in a way that does not require restrictions on the circuit's gate-set or the qubits' connectivity, e.g., as proposed

in [1], [2]. Also, they might also be used on the lowest possible level in order to perform noise-aware simulations which allow to estimate how a circuit is likely to perform on an actual device, e.g., as proposed in [19]–[21]. Either way, on both abstraction levels, quantum circuit simulation is non-trivial since corresponding representations of states and operations, in general, require exponential space or runtime—requiring powerful software tools.

Due to the immense complexity of the tasks involved in quantum circuit compilation (as it has been illustrated in Section II-A), e.g., mapping being NP-complete [22], manually conducting compilation often is not an option. Consequently, efficient software tools are needed across all levels of abstraction of the aforementioned flow in order to realize a conceptual algorithm on an actual device. Thus, various compilation tools have been proposed, e.g., [3]–[5].

During compilation, an algorithm's description is considerably altered and transformed. Naturally, it is of utmost importance to ensure that the originally intended functionality is preserved through all levels of abstraction. This procedure is called verification. While the underlying principle of comparing the transformations represented by different quantum circuits is conceptually simple, the exponential size of the underlying matrices makes this problem challenging—it has been shown to be QMA-complete [23]. Due to the increasing complexity of today's compilation flows, tools for verifying their results become increasingly important. Exemplary verification tools have been proposed in [6]–[10].

These design tasks demonstrate the wide variety of software tools operating on and across different levels of abstraction—leading to comprehensive quantum circuit design flows realized through toolkits such as IBM's Qiskit [11], Google's Cirq [12], or Rigetti's Forest [13]. At the same time, all these tasks have in common that they have an immensely large complexity. As such, a multitude of techniques for each task have been proposed—each with its own trade-off between resource demand and quality of the result. It is key in the development of scientific methods to empirically evaluate and compare their performances on practical, relevant benchmarks.

III. BENCHMARKING

The benchmark suite proposed in this paper is not the first and certainly not the last collection of quantum circuit benchmarks. In this section, we review some of the existing suites and their respective foci. Afterwards, we discuss how MQT Bench further complements this.

A. Current State of the Art

Providing a comprehensive set of benchmarks to satisfy the needs across all levels of the quantum circuit compilation flow is a challenging task. Several approaches to provide benchmark suites for some of the levels within the quantum circuit compilation flow have already been proposed and a non-exhaustive overview is given in the following:

Application-Oriented Performance Benchmarks for Quantum Computing [14]: Starting with an example located on the algorithmic level, this benchmark suite rather focuses on high-level descriptions. At the moment of writing, it provides 13 benchmark algorithms which can be generated with a variable number of qubits via jupyter notebooks using multiple software compilation flows and are classified into four categories of complexity. The resulting circuits are available as high-level Python objects without any further compilation steps.

QASMbench [15]: This benchmark suite focusses on the target-independent level. It offers numerous quantum circuits with a wide but fixed range of both the number of qubits and depth. It classifies the benchmarks into three categories of sizes and three categories of algorithm classes. All circuits are available in an intermediate representation according to the openQASM 2.0 specification [24].

SupermarQ [16]: Similarly to *QASMbench*, SupermarQ also focusses on the target-independent level with the contrast of providing benchmarks with adjustable qubit range for eight algorithms according to the openQASM 2.0 specification [24]. Additionally, six feature vectors are proposed to describe the characteristics of the benchmarks.

RevLib [17]: This benchmark suite provides a wide variety of reversible circuits in an intermediate representation format specified by the authors. Classical functions are frequently embedded into reversible circuits in order to use them in quantum algorithms, e.g., oracle functions or Boolean building blocks such as the modular exponentiation in Shor's algorithm [25]. In addition, decomposed versions of this benchmark suite have found widespread use in evaluating the performance of mapping tools, e.g., in [26]–[28]. Since reversible circuits merely form a subclass of quantum circuits and do not employ quantum mechanical effects such as superposition and entanglement, they do not serve as adequate benchmarks for the whole stack.

B. Motivation

All of the mentioned benchmark suites have in common, that they each target a specific abstraction level within the quantum circuit compilation flow. Although the respectively intended target level is well covered, the demand for a cross-level benchmark suite is not fully met yet. Additionally, so far, there is no mutual consolidation which benchmarks to use for empirical evaluations of software tools. This results in a lower comparability, reproduceability, and transparency of results and may even cause confusion because benchmarks believed to realize the same particular task are quite frequently realized in a completely different fashion, e.g., a benchmark called "grover" could realize Grover's algorithm with any particular oracle. Consequently, the demand for a benchmark suite spanning the whole stack of abstraction levels constitutes the main motivation of this contribution.

In order to realize such a benchmark suite, several challenges have to be tackled:

- Distinct requirements for benchmark circuits on different levels: The closer a level is to the actual computing hardware, the more requirements have to be fulfilled, e.g., only gates from the device's native gate-set are allowed and the connectivity of the hardware architecture must be considered.
- Accessibility: In order to facilitate its adoption, the benchmark suite needs to be as easy to use as possible. While most benchmark suites already provide open-source access, running and adapting the code to the user's needs, e.g., obtaining a selection of relevant benchmarks, frequently is tedious or impossible and a solution that keeps this hurdle low is desirable.
- Generalizability of a software tool: This can only be guaranteed if it is evaluated on a broad set of benchmarks, relating to several characteristics, e.g., the number of qubits, circuit depth, or the application domain.
- Extendability: Besides that, quantum computing is rapidly advancing and extendability of the benchmark suite to future algorithms, gate-sets, and architectures becomes even more important.

MQT Bench has been developed with these challenges in mind and aims to be a first step towards covering the whole quantum software stack with a benchmark suite based on the following four core traits (which are described in detail in Section IV):

1) Cross-level benchmarking: All benchmarks are provided on four abstraction levels reviewed in Section II-A.
2) Accessibility: A website to simplify the usage of MQT Bench as much as possible is provided (https://www.cda.cit.tum.de/mqtbench). While most needs of users should be covered by this, we additionally give access to the open-source repository on GitHub (https://github.com/cda-tum/MQTBench).
3) Algorithm Selection: Broad selection of different benchmarks with parameterizable characteristics ranging from building blocks, i.e., QFT, to applications, i.e., ground state estimation.
4) Extendability: MQT Bench is easily extendable regarding the available benchmarks, native gate-sets, and hardware architectures.

Benchmarking quantum software tools and compilation flows with the same benchmarks aims to aid comparability, reproducibility and transparency of empirical evaluations. How this leads to more consistent testing is shown in the following example.

Example 5. *Consider a full quantum compilation flow across all four levels which shall be developed and tested as depicted in Fig. 2. On the left-hand side of the levels, the current state of the art of benchmarking is sketched. To comprehensively test each level, different benchmark suites have to*
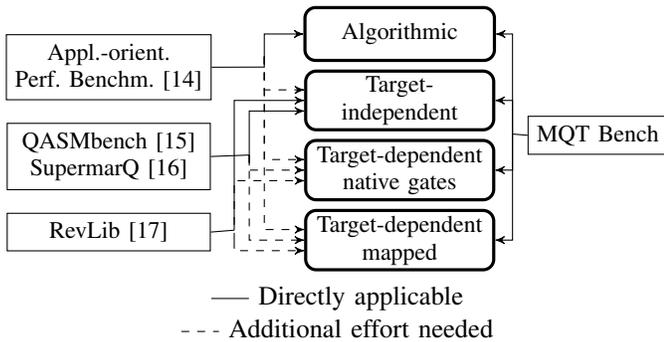
Fig. 2. Benchmarking software tools with and without MQT Bench.

be adapted and used. In contrast, MQT Bench replaces all of those and enables testing software tools with the same benchmarks throughout the whole quantum circuit compilation flow as shown on the right-hand side.

IV. MQT BENCH

In this section, we describe in more detail how each of the four previously mentioned core traits is implemented.

A. Cross-Level Benchmarking

As exemplarily illustrated in Section II, software development in quantum computing takes place at various levels. While there arguably are numerous possible levels, MQT Bench focusses on four as a balanced measure between specificity and generizability—inspired by the structure proposed in the openQASM 3.0 specification [18]. Providing these benchmarks on all of the four abstraction levels is the main contribution of this work. More precisely, the following levels are covered:

1) *Algorithmic level*: In this format, all kind of quantum gates may be used and subsumed into high-level building blocks. Loops are possible and the circuit structure might be described by constants, variables, and mathematical expressions. This level provides benchmarks on the most generic level and specific values are assigned to its variables, e.g., the number of iterations of a loop. The number of qubits can be specified through the MQT Bench web interface.

2) *Target-independent level*: Here, loop unrolling, constant folding and propagation are conducted. Also naive gate simplification is enforced. Again, the number of qubits can be adapted through the website.

3) *Target-dependent native gates level*: On this level, a particular native gate-set (e.g., IBM or Rigetti) is chosen, the circuit is transpiled accordingly and optimized. Here, the native gate-set and the optimization level can be specified.

4) *Target-dependent mapped level*: Finally, a dedicated architecture layout is chosen and the circuit is mapped to the targeted device so that it satisfies all its connectivity constraints and becomes executable on the device. In

addition to the specifiable parameters from the previous levels, two mapping schemes are provided. The benchmarks are either mapped to the smallest fitting or the largest possible target device regarding the number of qubits.

All relevant information of a generated benchmark are denoted in short in the file name and in detail within the file itself.

B. Accessibility

MQT Bench strives to fulfill the needs of many. In order to accomplish this goal, it has to be as user-friendly as possible. On the one hand, this involves the benchmark library itself. All of the high-level, algorithmic benchmark scripts and routines to generate representations for the individual levels are publicly available on GitHub (https://github.com/cda-tum/MQTBench). This allows for complete transparency on how the respective circuits have been generated.

On the other hand, and most importantly, this involves the way in which users interface with the benchmark suite. While most benchmark suites are provided as an accumulation of benchmark files—making it hard to extract the desired set of benchmarks, MQT Bench includes an easy-to-use, no-coding-required web interface (https://www.cda.cit.tum.de/mqtbench) that provides the means to filter the large number of pre-generated benchmarks according to the specific needs of the user. A screenshot of the website's user interface and its configuration options is shown in Fig. 3.

C. Algorithm Selection

To provide a broad spectrum of different benchmarks, MQT Bench comprises most of today's de-facto standard quantum algorithms. This includes building blocks, e.g., the Greenberger–Horne–Zeilinger state preparation (GHZ) or Quantum Fourier Transform (QFT), up to higher-level algorithms, e.g., Shor's [25] and Grover's [29] algorithm. At the time of writing, MQT Bench comprises the following benchmarks:

- GHZ state preparation
- Graph state preparation
- W-State preparation
- Amplitude Estimation (AE)
- Quantum Fourier Transformation (QFT)
- Quantum Phase Estimation (QPE)
- Deutsch-Jozsa (DJ) algorithm
- Harrow-Hassidim-Lloyd (HHL) algorithm
- Shor's algorithm
- Grover's algorithm
- Quantum Walk
- Quantum Approximation Optimization Algorithm (QAOA)
- Variational Quantum Eigensolver (VQE)
- Three VQA ansatz functions with randomly initialized parameters: Two Local, Real Amplitudes and Efficient SU2
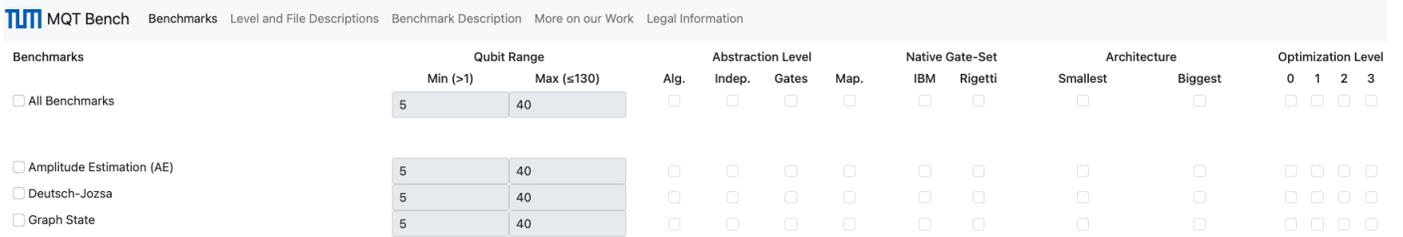
Benchmarks	Qubit Range		Abstraction Level				Native Gate-Set		Architecture		Optimization Level			
	Min (>1)	Max (≤130)	Alg.	Indep.	Gates	Map.	IBM	Rigetti	Smallest	Biggest	0	1	2	3
☐ All Benchmarks	5	40	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
☐ Amplitude Estimation (AE)	5	40	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
☐ Deutsch-Jozsa	5	40	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐
☐ Graph State	5	40	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐	☐

Fig. 3. User interface of the MQT Bench website. Due to the length of the benchmark listing, only the first three benchmarks are shown.

Additionally, MQT Bench provides several application benchmarks specifically targeting variational quantum algorithms, since those algorithms are especially promising in the NISQ-era [30]. To this end, we use the classification provided by IBM Qiskit's application levels: Optimization, Machine Learning, Finance, and Nature:

- *Optimization*: Travelling salesman problem and vehicle routing
- *Machine Learning*: Quantum Generative Adversarial Network (QGAN)
- *Finance*: Portfolio optimization and option pricing
- *Nature*: Ground and excited state estimation

D. Extendability

Quantum computing is a rapidly evolving area of research and, especially in the recent years, numerous promising algorithms and fields of application have emerged. Any benchmark suite has to be extendable and must continuously evolve in order to remain relevant. MQT Bench is designed to be easily extendable in a multitude of ways:

- *Benchmarks*: New applications and benchmarks can easily be integrated into MQT Bench by providing the corresponding algorithmic level description. The generation of all other levels and options (such as the native gate-sets, architectures, and optimization levels) is automatically handled by the proposed library.
- *Native gate-sets*: So far, the focus is on the native gate-sets of superconducting quantum computers developed by IBM and Rigetti. In the future, additional gate-sets (such as those of Google's and Oxford Quantum Circuits' superconducting processors or AQT's and IonQ's ion trap-based quantum computers) can be realized by adopting the necessary compilation routines in the proposed library.
- *Hardware architectures*: All major players currently rely on a modular platform for the architecture of their devices in order to further scale their quantum computers. It is straightforward to extend MQT Bench's list of available architectures to accommodate future architectures.

While the four levels MQT Bench is based on cover today's main use cases, the number of abstraction levels most likely is going to increase in the future. While the mapped level has mostly been considered the last one before a circuit is send to the quantum computer for execution, pulse-level programming is envisioned to give even more control to software developers as proposed in [31]. On the other end of the spectrum, higher-level abstractions and programming languages will be required to foster the adoption of quantum technology. Currently, a programmatic description for the benchmarks is needed on the algorithmic level. An even higher level where this programmatic description will be automatically derived from is also envisioned. *QUARK* [32], a framework for quantum computing application benchmarking consisting of four levels where the lowest level considers the whole compilation flow discussed in Section II-A, constitutes one step towards this direction.

V. CONCLUSION

In this work, we proposed *MQT Bench*—a quantum circuit benchmark suite comprising different algorithms, native gate-sets, and mapping schemes—resulting in more than 30.000 benchmark circuits ranging from 2 up to 130 qubits on four abstraction levels. To keep this large number of benchmarks manageable, we provide an easy-to-use web interface (https://www.cda.cit.tum.de/mqtbench) allowing users to filter the benchmarks according to their needs. Additionally, we give access to the open-source repository on GitHub (https://github.com/cda-tum/MQTBench). By this, *MQT Bench* presents a first step towards serving a single benchmark suite for the whole quantum software stack—facilitating empirical evaluations of quantum software tools that are comparable, reproducible, and transparent.

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