MorphQ: Metamorphic Testing of Quantum Computing Platforms

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ABSTRACT
As quantum computing is becoming increasingly popular, the underlying quantum computing platforms are growing both in ability and complexity. This growth may cause bugs in the platforms, which hinders the adoption of quantum computing. Unfortunately, testing quantum computing platforms is challenging due to the relatively small number of existing quantum programs and because of the oracle problem, i.e., a lack of specifications of the expected behavior of programs. This paper presents MorphQ, the first metamorphic testing approach for quantum computing platforms. Our two key contributions are (i) a program generator that creates a large and diverse set of quantum programs, and (ii) set of program transformations that exploit quantum-specific metamorphic relationships to alleviate the oracle problem. Evaluating the approach by testing the popular Qiskit platform shows that the approach creates over 50k program pairs within two days, many of which expose crashes. Inspecting the crashes, we find twelve bugs, eight of which have already been confirmed. MorphQ widens the slim portfolio of testing techniques of quantum computing platforms, helping to create a reliable software stack for this increasingly important field.

1 INTRODUCTION
Quantum software engineering is seeing an increasing interest from the research community and industry thanks to the continuous hardware improvements. Quantum computing platforms, such as Qiskit by IBM, Circ by Google, and Q# by Microsoft, are for this emerging field what traditional compilers and execution environments are for traditional programs. Ensuring the correctness of these platforms is crucial for the correct execution of quantum programs, whereas bugs in the platforms may undermine other advancements, such as in algorithms and hardware. A recent empirical study [21] has shown that quantum computing platforms are still plagued with bugs, many of which are due to quantum-specific bug patterns not present in traditional software. The increasing importance of these platforms hence calls for automated testing techniques targeted at them.

Effectively testing quantum computing platforms currently faces two important challenges. (C1) The first challenge is that there currently are only relatively few quantum programs, as the field is emerging and developers are only beginning to exploit its potential. From a testing perspective, this means that test inputs are a scarce resource. (C2) The second challenge is the well-known oracle problem [3], i.e., the problem of not having a specification of the expected behavior triggered by an input. In our context, the oracle problem is about determining what behavior the execution of a given quantum program should expose, which is particularly challenging since programs are composed of low-level operations, represented by gates, that translate to sometimes unintuitive and highly abstract operations on the inputs.

This paper presents MorphQ, the first metamorphic testing approach targeted at quantum computing platforms. The approach addresses challenge C1 by proposing the first automatic generator of quantum programs. The generator combines template-based and grammar-based code generation to produce programs that use a diverse set of quantum gates and options for compiling and executing them. To be effective, the generation must carefully consider domain-specific constraints typical of quantum computing, such as not applying any operation after a measurement gate because it would destroy the quantum state. MorphQ respects these constraints and generates valid programs, in the sense that they execute without crashing.

The approach addresses challenge C2 through a novel set of ten metamorphic transformations. Following the idea of metamorphic testing [6, 7], these transformations change a given source program into a follow-up program in such a way that the two programs have an expected output relationship, e.g., that they should expose the same behavior. If the expected output relationship does not hold, e.g., because the follow-up program crashes or otherwise exposes different behavior, the approach reports a warning. The metamorphic transformations are quantum-specific. For example, they change the order of qubits, add null-effect operations by exploiting the reversible nature of quantum computation, partition a circuit that contains unrelated subcircuits, or change the set of hardware gates a program is compiled to.

While testing tradition compilers has received significant attention [5], we are aware of only one piece of prior work, called QDiff [31], on automatically testing quantum computing platforms. MorphQ conceptually differs in multiple ways. One difference is that QDiff starts from a small set of manually written programs, whereas MorphQ generates a large and diverse set of quantum programs from scratch. Another difference is that QDiff is based on differential testing that compares executions with different optimization levels and backends, whereas MorphQ is the first to propose metamorphic transformations for quantum programs. Beyond conceptual contributions, we also empirically show our approach to complement prior work by finding bugs that previous testing work failed to find.

Our evaluation applies MorphQ to Qiskit [1], a popular quantum computing platform backed by IBM. Over a two-day testing period, the approach generates, executes, and compares over 50k pairs of quantum programs, many of which expose crashing bugs in the platform under test. Manually inspecting a subset of the warnings
reported by the approach, we find and report twelve bugs. So far, eight of them have been confirmed by the Qiskit developers. For example, these bugs are caused by incorrectly implemented optimization passes, missing support for specific kinds of programs, and mistakes in code that exports a program to QASM, an assembly-like language that allows for sharing quantum programs across different platforms. Studying the relative importance of our ten metamorphic relationships shows that each of them is involved in triggering at least some warnings reported by MorphQ and that applying multiple transformations in sequence is useful to detect otherwise missed bugs.

In summary, this work makes the following contributions:

- We introduce a novel template and a grammar, which represent valid quantum programs of the popular Qiskit platform.
- We introduce a template-based and grammar-based program generator that creates valid quantum programs to use for testing purposes.
- We design ten quantum-specific metamorphic relationships to enable the first metamorphic testing framework for quantum computing platforms.
- We integrate our approach with the popular Qiskit platform and provide empirical evidence that MorphQ reveals twelve real-world, crashing bugs.

Open science. Our implementation and all experimental results are being made freely available. 1

2 BACKGROUND ON QUANTUM COMPUTING

Unlike classical computing, which is based on classical physics, quantum computing exploits the laws of quantum mechanics to perform computation. Whereas in classical computing the minimal unit of information is a bit, which is either 0 or 1, in quantum computing the base unit is the qubit, which can be a superposition of 0 and 1 at the same time, representing a quantum state as $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$. This superposition is maintained and manipulated along the computation and at the very last stage, each qubit is measured and it results in either a 0 or a 1, with probability respectively $\alpha^2$ and $\beta^2$. Another important property is called entanglement, which means that the outcome of a measurement of two or more qubits shows some correlation.

1The code and data are available at the anonymous repo: https://anonymous.4open.science/r/MorphQ/
quantum programs, referred as source programs. Then by applying a sequence of one or more metamorphic program transformations, we derive a follow-up program that is in a specific relationship with the source program. Finally, the third step is to execute two quantum programs, compare their behavior, and check whether their behavior conforms to the output relationship expected for the input relationship. If the output relationship differs from the expected relationship, then MorphQ reports a warning to the user.

Algorithm 1 describes how MorphQ composes the three main steps. As input, the algorithm expects a program generator $G$, a set of metamorphic relationships $M$, and a component $C$ for comparing the behavior two quantum programs. Our approach is designed as a framework that allows for replacing and extending each component. The main loop of the algorithm continuously generates and checks new pairs of source and follow-up programs until running out of a configurable time budget. After each loop iteration, both programs are discarded, making each iteration independent from the previous one and preventing MorphQ from mutating previously crashed programs. Finally, the algorithm returns a set $B$ of pairs of programs that are likely to reveal a bug in the tested quantum computing platform.

As the first step in the main loop of the algorithm, the program generator $G$ creates a new quantum program $in_s$ using a combination of template-based and grammar-based code generation (line 3). A “program” here means source code that defines the quantum circuit and its execution setting, e.g., the type of backend to use or the transpiler’s settings. Then, the second step of the algorithm applies a sequence of transformations sampled from the metamorphic relationships $M$ to create a follow-up program $in_f$ (lines 4 to 15). Each metamorphic relationship has a precondition under which its transformation may be applied. Most of the transformations are designed to be semantically preserving, in which case the algorithm may continue to apply further transformations. The approach also includes two transformations that do not preserve the semantics, because they rearrange the qubits and execute only parts of the circuit to check some properties. Once such a transformation gets applied, the algorithm stops applying further transformations, which has the benefit that only the last transformation determines the expected output relationship. Finally, the third step compares the behavior of the source program $in_s$ and the final follow-up program $in_f$ (lines 16 to 19). The outcome of executing a program may be a program crash or non-crashing behavior. In the latter case, the platform repeatedly executes the circuit and summarizes the output into a distribution of bit-strings.

### 3.2 Program Generation

The first step of the approach generates quantum programs from scratch. A naive approach to this problem might consider all elements offered by the quantum programming language, e.g., all APIs offered by Qiskit, and combine them at random. However, such an approach would yield mostly invalid programs that crash and do not deeply test the platform. The reason is that quantum programs need to follow a particular structure and consider domain-specific constraints when combining the elements offered by the language.

The program generator in MorphQ is a combination of template-based and grammar-based code generation. The template-based part ensures that the created programs follow the typical structure of quantum programs, which is necessary to reach deep into the platforms under test. The grammar-based part is designed to cover a diverse range of possible programs by randomly combining gates with each other. The template and the grammar of our program generator are based on concepts available across different quantum
computing platforms, such as circuits, registers, gates and executing programs with a specific backend.

Figure 4 shows the template MorphQ uses to generate quantum programs. The placeholder `ALL_IMPORTS` gets replaced by the imports of all the dependencies used in a program. In the circuit section, the template creates a quantum register and a classical register of both of size `<N_QUBITS>`, and assembles them in a quantum circuit. The non-terminal `<GATE_OPS>` is expanded using the grammar described in Figure 5 to generate a valid sequence of gates, i.e., they act on some qubits in the available quantum and classical registers. Each instruction acts on a number of qubits between one and five, and contains a suitable gate that operates on them. The indices of the target qubits are selected randomly among the integers `<INT>` compatible with the maximum number `<N_QUBITS>` of qubits available. Each gate receives a specific number of parameters, which the generator chooses among the floating point numbers `<FLOAT>`. For brevity, Figure 5 shows only an extract of the whole grammar. Moving back to the template in Figure 4, in the transpilation section the generator replaces `<TARGET_GATE_SET>`, `<OPT_LEVEL>`, and `<COUPLING_MAP>` with two none placeholders. Finally, in the execution section of the program, it replaces `<BACKEND_NAME>` with a backend and selects the number `<N_SHOTS>` of shots to use in the execution. For determining the right number of shots to run the program, we use a sample estimation technique proposed in prior work [31].

Our implementation of MorphQ targets the Qiskit platform, which is highly popular and has been added also by previous work [12, 21, 38, 39], however we believe our approach could be easily extended to other quantum computing platforms. The generator supports a total of 45 gates, i.e., all but three gates expressible in Qiskit, excluded due to deprecation, presence of non-float parameters, or absence in the documentation. The 45 supported gates have up to four parameters and can act on up to five qubits. We limit the generation to maximum 30 consecutive gates to keep the execution time of programs within reasonable limits.

### 3.3 Metamorphic Testing Framework

A key technical contribution of MorphQ is a set of ten metamorphic relationships. We classify their corresponding transformations into three categories:

- **Circuit transformations**, which actively modify the circuit.
- **Representation transformations**, which change the intermediate representation used to represent the circuit.
- **Execution transformations**, which affect the execution environment, e.g., by changing the backend, the optimizer, the coupling map, or the target gates to use.

Table 1 summarizes all transformations. Some of them have a precondition, as checked at line 8 of Algorithm 1, which ensures that the resulting follow-up program is indeed expected to result in behavior described by a specific output relationship. All transformations in Table 1 are semantics-preserving, except for `Change qubit order` and `Partitioned execution`. For most of the transformations, the expected output relationship is equivalence, i.e., the source program and the follow-up program are expected to behave the same. We implicitly mean the output relationship to be equivalence, unless mentioned otherwise. In particular, this output relationships means that MorphQ reports a warning when the source program runs without crashing but the follow-up program produces a crash.

#### 3.3.1 Circuit Transformations

These transformations exploit the properties of the gate model of computation, such as the entanglement of qubits, the presence of registers and the properties of reversible computing.

**Change of qubit order.** Inspired by the bug pattern "incorrect qubit order" found in previous work [21], this transformation changes the order of qubits in the quantum register. Specifically, the transformation maps the qubit indices of source program to new positions and then creates a follow up program by adapting the sequence of gates to the newly mapped qubit indices. With reference to the
Table 1: Metamorphic relationships and their preconditions.

<table>
<thead>
<tr>
<th>Category</th>
<th>Name</th>
<th>Precondition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Circuit</td>
<td>Change of qubit order</td>
<td>-</td>
</tr>
<tr>
<td>transformation</td>
<td>Inject null-effect operation</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Add quantum register</td>
<td>Coupling map not fixed</td>
</tr>
<tr>
<td></td>
<td>Inject parameters</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Partitioned execution</td>
<td>Non-interacting subsets of qubits</td>
</tr>
</tbody>
</table>

| Representation transformation | Roundtrip conversion via QASM | - |
| Execution transformation     | Change of coupling map       | No added register                 |
|                              | Change of gate set           | -                                 |
|                              | Change of optimiz. level     | -                                 |
|                              | Change of backend            | -                                 |

grammar in Figure 5, the transformation hence consists in applying a bijective mapping between the \(\langle \text{INT} \rangle\) values of the source program and those of the follow-up program.

For example, consider the source circuit of Figure 6a, which has a two-qubit gate between qubit 1 and qubit 2. Applying the transformation with the qubit mapping \(m = \{0 \rightarrow 2; 1 \rightarrow 0; 2 \rightarrow 1\}\) results in Figure 6b, where the two-qubit gate now is between qubit 0 and qubit 1. The final measurement gates are not affected by the qubit mapping. Instead, the approach applies a function to all the output bit-strings of the follow-up program that applies the inverse of \(m\) to the order of measured qubits. In the example, suppose we obtain an output bit-string \(\phi_1\) by the follow-up program. The approach will turn it into a bit-string \(\phi_0\), because the bit at index 2 in the follow-up program corresponds to be at index 0 in the source program. After this re-mapping of the measurements, the two resulting output distributions are expected to be equivalent.

Inject null-effect operations. Quantum computing is an instance of reversible computing, i.e., performing any operation or gate, with the exception of the measurement gate, on a set of qubits never loses any information, and hence, can be reverted back with a suitable inverse operation. This metamorphic transformation exploits this property by inserting into the main circuit a sub-circuit that performs a sequence of gate operations followed by its inverse, so that the overall effect is null. Referring to the grammar in Figure 5, the transformation consists in injecting new code in between the sequence of gates generated by \((\text{GATE\_OPS})\). The sub-circuit may include an arbitrary number of gates and act on an arbitrary number of available qubits. The only restriction is that no measurement is introduced, because otherwise it would destroy the quantum state and change the result with respect to the source program. In our implementation, we limit the application of this transformation to program with a single main circuit, however in principle, it could also be applied with an arbitrary number of sub-circuits.

Figure 7 gives a concrete example of injected code. The inverse is produced via a function, typically called \(\text{inverse}\) (line 5), which is present on most quantum computing platforms and can be used to reverse the effect of a sub-circuit.

Add quantum register. Enlarging the set of available qubits by adding a new and unused quantum register should not affect the computation on the existing qubits. This transformation exploits this property by randomly adding new quantum registers to the circuit of the follow-up program. Referring to our template (Figure 4), the new register is added right before of after the measurement section, thus before the circuit is executed or even transpiled. This transformation cannot be performed when the coupling map has been specified before via the \(\text{Change of coupling map}\) transformation, since the addition of a register would make the coupling map too small.

Inject parameters. Given the recent interest in quantum machine learning, quantum computing platforms offer abstractions to support the parametrization of quantum circuits [24]. One of the sub-fields of quantum machine learning aims to use quantum circuits and the parameters of their gates as a quantum version of artificial neural networks [23]. This transformation creates such parameterized circuits by replacing one or more concrete floating point literals \(\langle\text{FLOAT}\rangle\) in the source program with a corresponding \(\langle\text{Parameter(\text{a})}\rangle\) object. Then, before the transpilation stage, the transformation binds all the free parameters to the original literal values of the source circuit. In analogy to non-quantum programs, this transformation resembles moving a literal value into a variable and then using the variable instead of the literal.

Partitioned execution. Some generated source programs might have two subsets of qubits that never interact with each other, i.e., there is no gate operation that involves the qubits of the two subsets. In this case, the source program performs two completely independent computations that can be executed in parallel. Given such a source program, this transformation separates the circuit into two sub-circuits, executes them individually, and then post-processes the result of the two sub-circuits to derive the distribution of the overall program.

The output distribution of the source program has bit-strings of size \(\langle\text{N\_QUBITS}\rangle\), whereas the result of the follow-up consists of two distributions with bit-strings of sizes \(a\) and \(b\), where \(\langle\text{N\_QUBITS}\rangle = a + b\). To reconstruct an output distribution of size \(\langle\text{N\_QUBITS}\rangle\) also for the follow-up program, the approach computes the Cartesian product of the output distributions of the two sub-circuits. That is, each individual bit-string of length \(a\) is concatenated to all bit-strings of length \(b\) to obtain the full output distribution of the follow-up program. More formally, the relationship between the output of the two sub-circuits and the output of the original source program is:

\[
U_s|\phi\rangle = U_{f_{\text{part1}}} |\phi_1\rangle \otimes U_{f_{\text{part2}}} |\phi_2\rangle
\]

where \(U_s\) represents the gates of the source program and \(|\phi\rangle\) represents all qubits, whereas \(U_{f_{\text{part1}}}\) and \(U_{f_{\text{part2}}}\) correspond to the two sub-circuits, and \(|\phi_1\rangle\) and \(|\phi_2\rangle\) are the two subset of qubits. The correct ordering of qubits is ensured by a mapping, similarly to the change of qubit order. In principle, this transformation can be applied to any arbitrary independent sets of qubits, our implementation focuses on two partitions for simplicity.

Figure 6c shows two separate partitions derived from the circuit in Figure 6a, the first partition with a single qubit and an “rx” gate, and the second with two qubits and the remaining gates.
3.3.2 Representation Transformations. We include in this category a transformation that acts on the representation of the quantum program, without affecting its computation or execution environment. We present one such transformation, but envision that others could be added for other intermediate representations of quantum programs.

**Roundtrip conversion via QASM.** OpenQASM [8], or short QASM, is the de-facto standard assembly language for quantum programs. Many quantum computing platforms offer API calls to convert to and from it. Although limited in its representational power, virtually all circuits can be expressed in the QASM format. Because correctly converting to and from QASM is an important prerequisite for the interoperability of quantum computing platforms, MorphQ comes with a transformation designed to exercise these parts of the platform under test. The transformation converts the quantum circuit to the QASM format and then parses the QASM code again to reconstruct the original circuit. Figure 8 shows the QASM code of the example in Figure 6a. To implement the roundtrip conversion in Qiskit, the transformation uses these API calls: `qc = qc_from_qasm_str(qc.qasm())`. The approach performs this transformation right before the execution section of the template in Figure 4, reflecting a realistic usage pattern of an interoperable format like QASM.

3.3.3 Execution Transformations. The third category of transformations is about adapting the execution environment. Given the currently available quantum hardware, called "noisy intermediate-scale quantum" (NISQ) devices [22], executing many generated programs on quantum hardware results in many noise-induced behavioral differences [31]. To avoid false positives caused by the limitations of today’s hardware, while still being able to find bugs in the software stack of quantum computing, MorphQ focuses on executing programs on simulators. We present four metamorphic transformations aimed at exercising the implementation of simulators, optimizations, and other aspects of executing quantum programs.

**Change of gate set.** During transpilation, a given quantum program is converted to be compatible with a specific target device, and this often involves translating the program gates to the natively supported gates. This transformation exercise this translation step by replacing the \( \langle \text{TARGET\_GATES} \rangle \) in the program template with a universal gate set, such as \( \langle \text{"rx", "ry", "rz", "p", "cx"} \rangle \) gates which has been shown to be universal [34]. This transformation considers three gate sets, however MorphQ easily supports the extension with other universal gate sets.

**Change of coupling map.** This transformation replaces the placeholder \( \langle \text{COUPLING\_MAP} \rangle \) in the program template with a randomly created coupling map to test whether the transpiler is able to adapt the quantum program to the new coupling map and still return an equivalent result. The coupling map represents the physical connections between bit pairs, and it is a simple list of pairs of integers. Note that MorphQ enforces the coupling map to be fully connected, i.e., no qubit is isolated, to ensure that every qubits can eventually interact with all the others at least indirectly via intermediate connections. An example of linear coupling map for our program in Figure 6a is: \( [[0,1],[1,2]] \), where the qubits 0 and 1 are connected with each other, whereas there is no connection between qubits 0 and 2.

**Figure 6: Examples of metamorphic transformations.**

(a) Source program.  
(b) Follow-up program after "change of qubit order".  
(c) Follow-up program after "Partitioned Execution".

**Figure 7: Example of code inserted by the “inject null-effect operation” transformation.**

```python
subcircuit = QuantumCircuit(qr, cr, name='subcircuit')
subcircuit.append(RXGate(6.12), qargs=[qr[0]], cargs=cr)
qc.append(subcircuit, qargs=qr, cargs=cr)
```

**Figure 8: Example of QASM code of Figure 6a.**

```qasm
OPENQASM 2.0;
include "qelib1.inc";
creg c0[3];
rx(pi) q0[2];
x q0[0];
h q0[1];
rx(pi) q0[2];
measure q0[0] -> c0[0];
measure q0[1] -> c0[1];
measure q0[2] -> c0[2];
```
Change of optimization level. The final two transformations are inspired by work on compiler testing [4]. One transformation replaces the \((OPT\_LEVEL)\) in the program template with another level between 0 and 3, which correspond to no optimization and heavy optimization. Similar to modifying the optimization level of a traditional compiler, this change is not expected to affect the final output of a program.

Change of backend. This transformation replaces the non-terminal \((BACKEND\_NAME)\) in the program template with another available backend. Different simulators typically have completely different implementations, such as one based on state vectors or density matrices. A single simulator often offers two variants, running on a CPU and GPU respectively, which we treat as two separate backends. In total MorphQ supports eight different backends. In analogy to testing traditional compilers, changing the backend roughly corresponds to comparing the behavior across different target platforms.

3.4 Comparing Execution Behavior
The third and final step of MorphQ is to execute both the source program and the follow-up program derived via our metamorphic framework, and to compare their behavior. If the two programs expose different behaviors, MorphQ adds them to the set of likely bug-revealing pairs of programs.

We perform this comparison at two levels. The first level identifies cases where one program runs without any crash, but the other program crashes. Our program generator (Section 3.2) is designed to create source programs that do not crash. However, applying the metamorphic transformations may trigger some bugs in the tested platform that manifest through a crash. We call pairs of a non-crashing and a crashing program a crash difference.

The second level applies when both programs run without any crash, where MorphQ compares the measured output bits. Due to the probabilistic nature of quantum programming, precisely comparing the output bit-strings would be misleading. Instead, the platform repeatedly executes each circuit for the specified number of shots and then returns the output distributions. MorphQ then compares the distribution of two programs. We use the Kolmogorov-Smirnov test [15, 26] to assess the statistical significance of the difference between the two distributions, as done in previous work [31], using a significance level of \(\alpha = 5\%\). We call any pair of programs with a \(p\)-value below \(\alpha\) a statistically significant distribution difference.

4 EVALUATION
Our evaluation focuses on the following research questions:

- RQ1: How many warnings does MorphQ produce?
- RQ2: What real-world bugs does the approach find in Qiskit?
- RQ3: How does MorphQ compare to prior work on testing quantum computing platforms [31].
- RQ4: To what extent do the different metamorphic relations contribute to the warnings and bugs found?
- RQ5: How efficient is MorphQ and what are the most time-consuming components?

Comparing the two kinds of differences that MorphQ reports during preliminary experiments, we find that crash differences typically point to actual problems in the tested platform, whereas distribution differences mostly correspond to false positives. The reason for the false positives is that the statistical test misreports distributions as different even though they are the same, which is expected to happen in a small percentage (\(\alpha\)) of all cases. As manually inspecting differences and understanding their root cause involves significant human effort, we focus our detailed evaluation on crash differences. An effective way to identify distribution differences that are likely true positives will be interesting future work, which then can be easily plugged into MorphQ.

To further motivate our focus on crash differences, we refer to the results of QDiff [31], i.e., the closest work existing work. Out of 33 divergent cases found by QDiff, the authors were able to spot and report bugs only for four crashing differences. All divergent cases due to distribution differences were attributed to possible hardware instabilities, which are frequent given the immature stage of real quantum computers.

4.1 Software Architecture and Extensibility
MorphQ is implemented in Python and tested on the latest Qiskit 0.19.1 version at the time of performing the evaluation. The implementation is designed in a modular way with four main components:

1. the MorphQ core, which is responsible for the orchestration of the various steps of the approach,
2. a program generator, which produces valid programs according to the API of the platform,
3. an extensible set of metamorphic transformations, which apply lightweight program transformations based on the API of the platform,
4. a divergence detector, which is responsible for spotting any distribution difference based on a statistical test by comparing the execution results. Note that only the program generator and the metamorphic transformations are platform-specific, whereas the MorphQ core and the divergence detector are cross-platform, making the approach modular and easily extensible. MorphQ currently supports Qiskit as a first target platform, but could be extended to other quantum computing platforms.

All experiments are run on a machine with 48 CPU cores (Intel Xeon Silver, 2.20GHz), two NVIDIA Tesla T4 GPUs with 16GB memory each, and 252GB of RAM, which is running Ubuntu 18.04.5.

4.2 RQ1: Warnings Produced by MorphQ
This research question evaluates MorphQ’s effectiveness at finding surprising behavior in a quantitative way. We run the approach for a total of 48 hours and summarize the results in Table 2. Over this period, the program generator produces a total of 50,591 programs.
All these program execute without crashing, which confirms that our template-based and grammar-based generation technique is successful at generating valid quantum programs. Applying metamorphic relations to these programs leads to a program crash in 29.0% of the cases, and hence, is reported as a crash difference. Out of the non-crashing executions, a small percentage of a total of 537 programs exposes a distribution difference.

**Answer to RQ1**: The program generation successively creates only valid quantum programs, and MorphQ is effective in producing numerous warnings by inducing 29.0% of all follow-up programs to crash.

### 4.3 RQ2: Real-World Bugs Found

To evaluate MorphQ's ability to find real-world bugs, we inspect a sample of warnings produced over a period of about 30 days. Because crash-inducing bugs are the most critical, as they impede developers from running their programs at all, and due to the difficulties in identifying true positives among the distribution differences, we focus our detailed inspection on crashing differences.

Before inspecting the program pairs, we semi-automatically cluster the warnings based on their crash message. To this end, we abstract program-specific references, such as line numbers, variable names, and file names, and then assign all warnings with the same abstracted message into a cluster. For example, "Duplicate declaration for gate 'ryy', line 4, fileA" and "Duplicate declaration for gate 'ryy', line 5, fileB" are assigned to the same cluster.

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Table 3 summarizes the results of our manual inspection. For each warning, we report the reference to the bug report\(^2\), its status, whether it was a new or duplicated bug report, the crash message, and what metamorphic transformation(s) are required to trigger the bug. Over the course of this study, we have filed a total of twelve bug reports in the Qiskit repository. So far, eight of the reports have been confirmed by the developers as bugs. The following describes some representative examples of the inspected warnings.

#### 4.3.1 Confirmed Bugs. Commutation analysis fails with \(\geq 11\) qubits (Bug 6).

This bug is detected thanks to two different metamorphic transformations applied simultaneously, showing the importance of combining multiple transformations. The transformations involved are: *change of optimization level* and *inject null-effect operations*. Figure 9 shows the minimized follow-up program consisting of a main circuit with eleven qubits, a subcircuit with ten qubits, and an optimization pass of level 2. This program triggers a generic Numpy error message. As confirmed by a Qiskit developer, the bug is in a specific analysis part of the optimization, called the *CommutationAnalysis*. The goal of this analysis is to find operation nodes that can commute in the direct acyclic graph representing the program. The problem is that the implementation of this analysis relies on matrix multiplications with \(n\_qubits \times 3\) dimensions, which in the case of eleven qubits is 33, whereas the maximum dimension supported by Numpy is 32 (numpy.MAXDIM).

**Identity gate hinders gate conversion (Bug 1)**. This bug is discovered by the transformation *Change of gate set*. Whenever the transpiler has to convert a circuit that, among the other gates, includes an identity gate, then the transpiler fails. The reason is that the identity gate is treated as a delay by the scheduler, since an identity gate operation is equivalent to a no-operation. As a consequence, there is no translation rule for the identity gate which leads to an exception in the translation process. The developers confirmed the bug, which had already been detected independently, and proposed a patch to fix it.

**QASM exporter creates invalid output for subcircuits with classical registers (Bug 8)**. This bug is triggered by a combination of two transformations: *Roundtrip conversion via QASM* and *Inject null-effect operations*. Figure 10 shows a minimized circuit that triggers the bug. It contains a subcircuit with a classical register, which is then converted to QASM and back to a quantum circuit. Running this code makes the QASM importer call to *qasm_from_str* produce an error caused by parsing invalid QASM code. The root cause of the error is actually in the QASM exporter, which produces the faulty QASM code shown in Figure 11. A Qiskit developer confirmed this bug by saying it should have been rejected by the exporter, since it is not possible to represent sub-circuits with classical registers in QASM.

#### 4.3.2 False Positives. Beyond actual bugs, MorphQ may also report false positive warnings in case the assumptions of our metamorphic relations do not hold. We are aware of one such case, which

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\(^2\)Removed for double-blind review. See supplementary material for anonymized versions of the bug reports.
Table 3: Real-world bugs and warnings found by MorphQ.

<table>
<thead>
<tr>
<th>ID</th>
<th>Report</th>
<th>Status</th>
<th>Novelty</th>
<th>Crash message</th>
<th>Metamorphic transformations</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>#7641</td>
<td>confirmed</td>
<td>duplicate</td>
<td>Instruction id not found</td>
<td>Change of gate set</td>
</tr>
<tr>
<td>2</td>
<td>#7326</td>
<td>confirmed</td>
<td>duplicate</td>
<td>Mismatch between parameter binds</td>
<td>Inject parameters</td>
</tr>
<tr>
<td>3</td>
<td>#7756</td>
<td>confirmed</td>
<td>duplicate</td>
<td>Cannot find gate definition for ‘c3sx’</td>
<td>Roundtrip conversion via QASM</td>
</tr>
<tr>
<td>4</td>
<td>#7749</td>
<td>confirmed</td>
<td>duplicate</td>
<td>Duplicate declaration for gate ‘rxx’</td>
<td>Roundtrip conversion via QASM</td>
</tr>
<tr>
<td>5</td>
<td>#7694</td>
<td>confirmed</td>
<td>new</td>
<td>qargs not in this circuit</td>
<td>Change of optimization level, Change of coupling map</td>
</tr>
<tr>
<td>6</td>
<td>#7700</td>
<td>confirmed</td>
<td>new</td>
<td>too many subscripts in einsum (numpy)</td>
<td>Change of optimization level, Inject null-effect operations</td>
</tr>
<tr>
<td>7</td>
<td>#7748</td>
<td>confirmed</td>
<td>new</td>
<td>Cannot bind parameters not present in the circuit</td>
<td>Inject parameters</td>
</tr>
<tr>
<td>8</td>
<td>#7750</td>
<td>confirmed</td>
<td>new</td>
<td>Gate or opaque call to ‘subcircuit’</td>
<td>Roundtrip conversion via QASM, Inject null-effect operations</td>
</tr>
<tr>
<td>9</td>
<td>#7769</td>
<td>reported</td>
<td>-</td>
<td>Cannot find gate definition for ‘rxx’</td>
<td>Roundtrip conversion via QASM, Inject null-effect operations</td>
</tr>
<tr>
<td>10</td>
<td>#7771</td>
<td>reported</td>
<td>-</td>
<td>Duplicate declaration for gate ‘ryy’</td>
<td>Roundtrip conversion via QASM, Inject null-effect operations</td>
</tr>
<tr>
<td>11</td>
<td>#7772</td>
<td>reported</td>
<td>-</td>
<td>Cannot find gate definition for unitary</td>
<td>Change of optimization level, Roundtrip conversion via QASM, Inject null-effect operations</td>
</tr>
<tr>
<td>12</td>
<td>#7773</td>
<td>reported</td>
<td>-</td>
<td>Cannot find gate definition for ‘rcccx’</td>
<td>Roundtrip conversion via QASM, Inject null-effect operations</td>
</tr>
</tbody>
</table>

Figure 11: Wrong QASM code produced because of Bug 8.

happens during the Change of gate set transformation. The transformation assumes that any circuit can be transformed into an equivalent circuit that uses only gates inside one of the universal gate sets. While this assumption holds in theory, the implementation in Qiskit uses the A* algorithm to find an equivalent sequence of gates because exploring all possible sequences is computationally expensive and impractical. Because this search may fail in the computational budget provided by Qiskit, the follow-up program sometimes crashes with a "Unable to map source basis to target basis" crash message, which does not point to a bug in the platform, but simply a limitation of its implementation.

Answer to RQ2: MorphQ has discovered twelve bugs in the latest version of Qiskit, eight of which have already been confirmed by the developers.

4.4 RQ3: Comparison with Prior Work

We compare with QDiff [31], which is the only other automated technique for testing quantum computing platforms that we are aware of, by comparing to the results reported in their paper. For a fair comparison, RQ1 uses the same approach as in their work, i.e., to measure the number of warnings produced in a fixed time budget. Like in their evaluation, we set the time budget to two days. During its evaluation on Qiskit, i.e., the target platform of our evaluation, QDiff has reported distribution differences due to hardware characteristics, not software bugs. In contrast, MorphQ has discovered several software bugs in Qiskit, as described in detail in RQ2. None of the bugs reported in Table 3 has been found by QDiff.

Answer to RQ3: MorphQ has revealed new bugs not found by prior work [31], showing that it complements the state of the art.

4.5 RQ4: Contribution of Metamorphic Transformations

To better understand to what extent the different metamorphic transformations in MorphQ contribute to its effectiveness, we check which transformations are involved in reporting warnings. We address this question from a qualitative and a quantitative perspective. For a qualitative answer, the last column in Table 3 shows for each of the manually inspected warnings which metamorphic transformations are essential to expose the unexpected behavior. Finding these twelve warnings involves a total of six metamorphic transformations. The most prevalent transformation is Roundtrip QASM conversion. We also find that seven out of the twelve warnings require at least two transformations, underlining the importance of combining them.

From a more quantitative perspective, Figure 12 reports the metamorphic transformations involved in the 50,591 pairs of programs from RQ1. For each transformation, the figure shows how many program pairs with that transformation exhibit the same behavior, a crash difference, or a distribution difference. If a pair is the result of applying multiple transformations in sequence, we count it multiple times. The transformation leading to most crashes is Change of gate set, which leads to the false positive discussed in Section 4.3.2. The second highest crash-inducing transformation is Roundtrip QASM Conversion, which shows that QASM exporter and importer is a...
complex, error-prone component of the platform under test. Inject null-effect operations and Inject Parameters also induce a sizable set of crashes, which we attribute to the fact that they exercise recently added code. Notably, each of the transformations leads to at least some unexpected behavior, showing that they all contribute to the overall effectiveness.

**Answer to RQ4:** All the metamorphic transformations in MorphQ contribute to detecting unexpected behavior, and often more than one transformation is needed to detect a warning.

### 4.6 RQ5: Time Cost per Component

The following studies how efficient the different steps of MorphQ are and which step takes most time. We measure the time spent in the three main components, namely (i) generating source programs, (ii) creating follow-up programs via a series of transformations, and (iii) executing programs on simulators and compare their behavior. Figure 13 reports the time per component, on average for a single pair of programs, during the two-day experiment from RQ1. The by far most time-consuming step is to execute the programs, as executing larger circuits in a simulator running on classical hardware is known to be slow. In contrast, generating and transforming programs take only 6.2ms and 30.6ms, respectively.

**Answer to RQ5:** Program generation and performing metamorphic transformations are efficient, together taking only 36.9ms per program pair, whereas executing the programs on simulators is the most time-consuming step of the approach.

### 5 THREATS TO VALIDITY

There are some threats to the validity of our results and the conclusions to draw from them. First, the results might be influenced by the non-deterministic, randomized nature of the program generator and the selection of transformations. We mitigate this threat via long-running experiments, which compensate for any bias in the results one might observe with only a few generated programs. Second, the number of warnings gives only a partial view of the effectiveness of MorphQ due to the presence of duplicates [4]. To mitigate this threat we cluster warnings and inspect a sample, showing that there are at least twelve unique bugs. Finally, our experiments focus on a single target platform and we cannot claim that our results will generalize beyond it. We believe the approach could also be applied to other quantum computing platforms that use a circuit-based computational model, provide similar programming abstractions, and offer QASM compatibility, such as Pytket [25] and Cirq [9].

### 6 RELATED WORK

**Quantum computing platforms.** A study by Paltenghi and Pradel [21] identifies ten quantum-specific bug patterns in quantum computing platforms, such as incorrect qubit order and incorrect intermediate representation, which inspired some metamorphic transformations of MorphQ. Another study [39] gathers a dataset of 36 bugs in Qiskit and identifies crashes and wrong outputs as the most common manifestation of bugs, which is exactly what MorphQ focuses on. Sodhi and Kapur [27] study quality attributes of these platforms and discuss challenges faced by platform developers. All these studies motivate work on testing quantum computing platforms. Prior to our work, there has been only one other approach addressing this challenge [31] (see Section 4.4 for a detailed comparison), showing that MorphQ addresses an important problem.

Wang et al. [31] propose QDiff, a differential testing technique for quantum computing platforms. In contrast to our work, QDiff does not generate programs from scratch, but starts from six hand-written programs. Moreover, QDiff performs differential testing across different backends and optimization levels of quantum computing platforms, whereas our work is based on a novel set of metamorphic transformations, only two of which (change of optimization level and change of backend) are similar to QDiff. See Section 4.4 for our empirical comparison with QDiff.

**Testing and manipulating quantum programs.** A problem related to that addressed here is how to test quantum programs. Several approaches have been proposed, including a search-based techniques [30, 33], statistical assertion checks that try to limit the effects on the actual computation [14, 18, 19], combinatorial testing [32], and coverage-based methods [2]. In contrast to our work, these techniques test specific programs, not the platform that programs are running on. CutQC [28] breaks a quantum circuit into smaller parts so that the resulting sub-circuits can be executed on the limited NISQ devices [22]. Our partitioned execution transformation also splits a circuit in sub-circuits, but only when the qubits are not entangled, whereas CutQC handles entanglement by classical postprocessing that approximates the output distribution. Thus, unlike CutQC, our transformation does not introduce any approximation.
Testing of probabilistic systems. ProbFuzz [11] is a testing technique targeted at probabilistic systems, such as probabilistic modeling libraries. While both those libraries and quantum computing platforms output probabilistic distributions, the latter is more deeply connected to hardware constraints, e.g., via a coupling map and the gate set, which our approach considers.

Testing compilers and other developer tools. The critical role of compilers for overall software reliability has motivated a stream of work on compiler testing. We refer to a recent survey [4] for a comprehensive overview. Quantum computing platforms play a similarly critical role in the quantum computing domain, which motivates our work. Our program generator relates to work on generating traditional programs, e.g., via randomized code generation combined with static and dynamic checks to avoid undefined behavior [35], code fragment-based fuzzing [13], and systematic program enumeration [37]. Metamorphic testing has also been applied in compiler testing, e.g., by deleting and inserting code in the dead regions of a program [16, 17], and via domain-specific transformations for graphics shading compilers [10]. Other developer tools, e.g., debuggers, can also be subject to metamorphic testing [29]. None of the above approaches addresses the unique challenges of quantum computing platforms, for which MorphQ contributes a novel program generator and a novel set of metamorphic transformations.

7 CONCLUSION

Motivated by the increasing popularity of quantum computing paired with the slim portfolio of techniques for testing its software stack, this paper presents the first metamorphic testing approach for quantum computing platforms. Our two key contributions are a program generator that efficiently creates a diverse set of non-crashing quantum programs, and a novel set of metamorphic transformations to create pairs of programs to compare with each other. Our evaluation shows MorphQ’s effectiveness, e.g., in the form of twelve detected bugs in Qiskit. We envision our two key contributions to enable future work beyond MorphQ. For example, the program generator provides a starting point for other testing techniques, e.g., coverage-guided fuzzing, and the metamorphic transformations could be adapted to other platforms. Overall, the presented work takes an important step toward further increasing the reliability of software in this still young field.

REFERENCES


