CertiQ: Contract-based Verification of a Realistic Quantum Compiler

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Abstract

In this paper, we present CertiQ, a mostly-automated verification framework for the Qiskit quantum compiler. CertiQ, to our knowledge, is the first effort enabling the automated verification of a realistic quantum program compiler. Qiskit is currently the most widely-used open-source quantum software stack from low-level compilation to high-level quantum algorithms. With growing community contributions, the Qiskit compiler is in need of code quality control and verification down to the compilation level to guarantee reliability of scientific work that uses it. CertiQ is deeply integrated into the Qiskit compiler, providing abstract specifications for quantum compiler data structures and offering verifiable contracts that specify the behaviors of compilation phases with heavy optimizations. CertiQ enables the verification of the current implementation of the Qiskit compiler and future code submissions in a mostly-automated manner using invariant-guided contracts to scale the symbolic reasoning. With these CertiQ techniques in place, developers need to provide limited inputs only where function contracts and loop invariants cannot be inferred automatically. The CertiQ verification procedure discovers several critical bugs, some of which are unique to quantum software. Our extensive case studies on four compiler phases of Qiskit demonstrate that CertiQ is effective for verification of quantum compilers with a low proof burden.

1 Introduction

The development of NISQ [32] (Noisy Intermediate-Scale Quantum) devices has transformed quantum computing from an academic pursuit to a realistic goal for the realization of practical quantum applications. NISQ devices like IBM's quantum machine with 20 qubits and Rigetti's quantum machine with 19 qubits has led to the emergence of cloud-based quantum services and associated computing software stacks [1, 6, 34].

Qiskit [1] is currently the most complete and widelyused open-source software stack. Qiskit lets users design and run quantum programs on the IBM Q cloud [20], a cloud based service for near-term quantum computing applications and research. With more than 100K users from 171 countries, Qiskit has accommodated over 5.3M experimental runs on quantum devices and 12M virtual simulations to date. Qiskit is also influential in the opensource community: with 180k downloads, 1500 Github forks (with 2nd place Cirq [6] < 500) and Github "usedby" of 122 (with 2nd place Qutip [37] with 59). Over 190 academic articles are based on IBM's cloud service, pushing progress in many different scientific disciplines, including: validation of properties of electron structure [45]; demonstration of error detection schemes [50]; demonstration of quantum machine learning algorithms [41, 54].

The increasing numbers of quantum computations have revealed numerous errors at all levels in the Qiskit toolchain, which can corrupt the scientific results performed with it. Specifically, the different nature of quantum computations along with heavy optimizations performed in the Qiskit compiler (called Qiskit Terra) makes the compilation error-prone. The high number of bug reports [48] related to the compilation process highlights the crucial need for effective, reliable, and automated methods to verify the correctness of quantum compilers with heavy optimizations.

We introduce CertiQ, a mostly-automated framework for verifying that a quantum compiler is correct, i.e., the compiled quantum circuits will always be equivalent to the source circuits. To our knowledge, CertiQ is the

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first effort enabling the automated verification of a realworld quantum program compiler. The design philosophy underpinning CertiQ is motivated by three practical challenges that arise when verifying Qiskit Terra.

The first challenge is that checking the equivalence of quantum circuits is generally intractable [21]. To mitigate this problem, CertiQ introduces the *calculus of quantum circuit equivalence* such that circuit equivalence and the correctness of compiler transformation can be statically and efficiently reasoned about. Our calculus is proven to be sound and therefore faithful to the underlying quantum computation. Based on the calculus, we design, specify, and verify a library of functions that perform primitive circuit transformations that are proved to be semantics preserving. Compilation phases implemented with this library can be easily verified using symbolic reasoning [12].

The second challenge is that compiler implementations in community code submission can be complicated, making automated verification intractable due to state explosion. In CertiQ, we developed a novel way of combining symbolic execution and Design-by-Contract methodology to achieve high level of automation and scalable verification. CertiQ first re-direct the code to be verified to the verification backend, built upon the push-button verification framework [31, 44], then uses symbolic execution to generate verification conditions in the form of satisfiability modulo theories (SMT) problems fed into a SMT solver, e.g., Z3 [11]. For more efficient symbolic execution, CertiQ offers three Z3 predicates/functions (that return the precondition, postcondition and invariants, respectively) as a contract for each library function and each transpiler pass. During the symbolic execution, invocations of functions that have been verified are replaced by their contracts. In this way, CertiQ is able to greatly speed up the symbolic execution and reduce the size of the generated SMT queries. This usage of contracts can be viewed as *predicate abstraction* [8, 16], where our domain knowledge of the quantum data structures is used to simplify concrete predicates.

The third challenge is that the different nature of quantum computation can cause unexpected behavior of components when interacting with each other in a large and rapidly growing quantum software. Specifically, in Qiskit, there exist multiple quantum data structures representing the same underlying quantum object, i.e., state vector representation and Bloch sphere representation of qubits. CertiQ verifies the equivalence of these quantum data structures through *specification refinement* and specifies the conditions under which each of these data structures are valid.

For important types of compiler extensions (optimizations), if an implementation by developers cannot be verified by the CertiQ verifier, CertiQ introduces a translation validator to validate the correctness of each compilation output at runtime with reasonable overhead.

We verified four compiler phases and seven transpiler pass implementations of Qiskit Terra in four case studies. With these verified CertiQ implementations, we successfully identify three bugs of Qiskit Terra, two of which are unique in quantum software.

This paper makes the following contributions:

- We introduce the calculus of quantum circuit equivalence such that the semantics-preserving guarantee of quantum circuit compilations can be statically and efficiently verified.
- We build a transformation library verified with respect to its contract, which guarantees that the provided circuit transformations preserve the circuit equivalence. This library can be used to build verified quantum compilers.
- We introduce a contract-based design that specifies the behavior of other functions, thereby facilitating efficient symbolic execution and modular verification of quantum compiler implementations.
- We used specification refinement to prove the equivalence of quantum data structures and regulates the transformation between them.
- We verify a series of Qiskit Terra compilation phases and optimizations, and discover three critical bugs. Two of these bugs are unique to quantum software.

The paper is organized as follows: §2 introduces background on quantum computing and Qiskit Terra; §3 provides an overview of the CertiQ framework; §4 discusses technical contributions of CertiQ; §5 presents case studies demonstrating how CertiQ works in the realistic settings; §6 evaluates the correctness and performance; §7 discusses previous work; §8 concludes.

2 Background

2.1 Quantum Computing

Principle of quantum computation. The qubit (quantum bit) is the basic element of a quantum computing system. In contrast to classical bits, qubits are capable of living in a superposition of the logical states $|0\rangle = 1, 0^T$ and $|1\rangle = 0, 1^T$. The general quantum state of a qubit is represented as $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ (or in its vector form α, β^T), where α, β are complex coefficients with $|\alpha|^2 + |\beta|^2 = 1$. When measured in the 01 basis, the quantum state collapses to $|0\rangle$ or $|1\rangle$ with probability of $|\alpha|^2$ and $|\beta|^2$, respectively.

The number of quantum logical states grows exponentially with the number of qubits in a quantum system. For example, a system with 3 qubits lives in the superposition of 8 logical states: $|000\rangle$, $|001\rangle$, $|010\rangle$, ..., $|111\rangle$. This property sets the foundation of quantum speedup



Fig. 1. Examples of circuit decomposition: SWAP gate decomposition (left); A circuit for preparing the 3 qubit GHZ state: $|\psi_{\text{GHZ}}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$. (right).

over classical computation—an exponential number of correlated logical states can be stored and processed simultaneously by a quantum system with a linear number of qubits. However, this also brings great challenges for simulating and verifying quantum computations.

Quantum gates. The basic quantum operations are called quantum gates, which are unitary transformations on the qubit space. Some of the quantum gates commonly used in quantum algorithms include X gate, Y gate, Z gate, H gate, T and CNOT gate.

2.2 Compilation of Quantum Programs

Quantum compilation is the process of translating highlevel description of quantum algorithms to a circuit consisting of a series of quantum gates. Such a compilation process can be divided into four stages: 1) circuit decomposition; 2) system-independent optimization; 3) technology mapping; and 4) system-dependent optimization.

In the first stage, quantum algorithms are decomposed into quantum circuits. Figure 1 illustrates two simple examples of circuit decomposition: decomposition of a SWAP gate to 3 alternating CNOTs; decomposition of the circuit for preparing the 3-qubit GHZ state $|\psi_{\text{GHZ}}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$ with CNOT and Hadamard gate, a quantum state used widely in quantum computation and communication. The system-independent optimization stage (stage 2) involves post-decomposition optimizations like circuit rewriting[46], template matching [27], commutativity detection [43].

Stage 3 technology mapping makes sure that the decomposed quantum circuit conforms to the topological constraints of the QIP platform. This process is usually executed by introducing quantum SWAP gates into the circuit.

The system-dependent optimization stage 4 further decomposes the gate set used in quantum algorithms to the gate set that can be executed on the QIP platform. Stage 4 also performs optimizations like single qubit rotation merge [9].

2.3 The Qiskit Terra Compiler

The Qiskit Terra compiler is the foundation of the Qiskit framework, upon which other Qiskit components are built. Qiskit Terra consists of a set of tools for composing quantum programs at the level of circuits, optimizing



Fig. 2. Qiskit Terra components and call graph. Green boxes are quantum data structures. Blue boxes are physical devices related data structures. The red box is the transpiler. CertiQ gives specifications to components in blue and green boxes and verifies the transpiler in red box. White boxes under the horizontal dotted-line are parts that are not verified or just partly verified by CertiQ.

them for the constraints of a particular physical quantum processor, and managing the batched execution of experiments on remote-access backends. The optimizations in Qiskit Terra are crucial for successful execution of quantum programs since quantum resources are scarce and qubit coherence time is very limited.

We describe the main components of the Terra compiler (Fig. 2), to which the CertiQ framework provides abstract specifications and contracts.

Quantum register. A quantum register is a collection of qubits that provides certain functionality in a quantum algorithm. Every qubit lives in a quantum register.

Coupling map and layout. Coupling map is the description of the connectivity of qubits on the physical device.



Fig. 3. The DAGCircuit representation of the circuit that prepares the GHZ state(See also Fig. 1 on the right). Green nodes are input nodes, blue nodes are operation nodes and red nodes are output nodes. Arrows represent dependency and are specified by qubit number. DAG representation is equivalent to a quantum circuit description, thus, throughout the paper we will use circuit diagram for visualization for readability.

It stores the edges of the qubits in a list. For example, coup = [[0,1], [1,2], [2,3]] describes a device of 3 physical qubits with linear connectivity. A layout is a Python dictionary from the virtual qubits in the quantum register to the physical qubits on the device. For example, the implementation in Terra is,

```
class Layout():
    def __init__(self):
        self._p2v = dict() # Physical to virtual qubit map
        self._v2p = dict() # Virtual to physical qubit map
```

QuantumCircuit. QuantumCircuit is the class that stores quantum circuits as a series of instructions on classical and quantum registers. It provides an interface to input quantum circuit description and for visualization.

DAGCircuit. The DAGCircuit class is another description of a quantum circuit and is equivalent to QuantumCircuit. Compared to QuantumCircuit description, DAGCircuit provides more flexible APIs for circuit transformations and to explicitly express the dependence between individual gates in circuits. For example, it provides a method topological_op_nodes() that allows users to traverse gates in the DAG in topological sort, easing out lots of circuit optimization algorithms.

Transpiler. The transpiler is the circuit rewriting module in Qiskit Terra responsible for stage 2, 3, and 4 in the quantum compilation process. Because transpiler is the critical part of the compiler and also the fastest iterating component, the need for automated verification is thus pressing. The design language of the transpiler is similar to that of LLVM [23]. It consists of modular components called transpiler passes that can be assembled by the transpiler pass manager with respect to their dependency constraints. Input and output of transpiler passes are both DAGCircuit. There are two classes of passes: analysis passes and transformation passes. Analysis passes compute useful quantities for the input DAGCircuit while preserving the DAGCircuit. Transformation passes performs circuit optimization or constraint resolving on the DAGCircuit, either returning the modified DAGCircuit or returning a new DAGCircuit.

3 The CertiQ Workflow

To give an overview of the CertiQ framework (Fig. 4), we walk through the verification of a simple and less "quantum" transpiler pass. The verification engine of CertiQ consists of four parts: specifications for Qiskit Terra quantum data structures/transformations, the verifier, the visualizer, and the translation validator. The core part is the CertiQ verifier, which builds upon the push-button verification framework in classical computing [31, 44]. We use a simple transpiler pass named



Fig. 4. The workflow of CertiQ framework. Blue boxes indicate CertiQ component. User code can be executed at two different backends. The usual Python backend and the verification engine share the same unified interface. In most cases, the user can be unaware of the verification engine when writing code.

basic-swap as a running example to introduce each of the parts.

3.1 The BasicSwap pass.

First, we look into the implementation of the BasicSwap pass (see Fig. 5). This pass serves as the benchmark for a large class of important transpiler passes that perform swap gate insertion. Swap insertion passes bring the qubit operands together for every 2-qubit gates in a circuit so that the 2-qubit gate operations can be done physically in two *connected* qubit locations on the coupling map. BasicSwap pass first generates an initial mapping for the qubits in the circuit (called layout), then it takes a simple algorithm that iterates all the 2-qubit gates in a circuit and move 2 operands of the 2-qubit gates together along a shortest path on the coupling map. When invoked, the ___run_() method of BasicSwap class takes a DAGCircuit as input and returns a mapped DAGCircuit as output.

3.2 Specifications

As shown in Fig. 4, when the verification engine is toggled on, the code of **BasicSwap** pass (or more generally, user implementations) will not go through the Qiskit backend, but the CertiQ backend instead. All the function calls and class invocations to the Qiskit library will be directed to its Z3 implementations in CertiQ. These alternative implementations in CertiQ can be viewed as

```
# @swap
class BasicSwap(TranformationPass):
  def ___init__(self, layout=None, coupling_map):
     self.layout = layout
     self.coupling_map = coupling_map
  def __run__(self, dag):
    if self.layout == None:
      self.layout = simple_layout(dag.greg,
                                  self.coupling_map)
    # Traverse the dag
    for gate in dag.topological_op_nodes():
      if gate.op_num == 2:
        p1 = self.layout[gate.op1]
        p2 = self.layout[gate.op2]
        s_path =self.coupling_map.shortest_path(p1, p2)
        for i in range(len(s_path)-1):
          dag.swap_and_update_gate(i, i+1)
    return dag
```

Fig. 5. Implementation of the BasicSwap pass.

specifications of quantum data structures and library functions in Qiskit Terra. These specifications share the same interface with the original implementation and are statically verified against them (this is detailed in §4.3). Importantly, specifications in CertiQ support symbolic execution. There are two kinds of specifications: *trusted specifications* and *abstract specifications*.

Trusted specifications. For example, the specification of the Layout class called in BasicSwap is a trusted specification. The specification of Layout class is,

```
class Layout(): # Layout specification
  def __init__(self):
    # Physical to logical qubit map spec
    self._p2v = Map(IntSort(), IntSort())
    # Logical to physical qubit map spec
    self._v2p = Map(IntSort(), IntSort())
```

In this case, the specification in CertiQ is almost identical to the Layout implementation in Terra (see §2.3) with the only difference that Layout specification uses Z3 Map rather than Python dict. Here, we include Map Z3 in our Trusted Computing Base (TCB) and trust that it correctly specifies dict in Python.

Abstract specifications. For more complicated data structures, for example, DAGCircuit, we need to use abstract specifications for the ease of symbolic execution and verification. The abstract specification of the DAGCircuit class is an array of gates,

The equivalence between all abstract specifications and their implementations is verified using *specification* refinement (see $\S4.3$).

3.3 Contracts and verification goals

The concept of contract is deeply rooted in the design of CertiQ. In CertiQ, a contract consists of three Z3 functions: the pre-condition function, the post-condition function, and the invariant function. Each of these functions takes Z3 variables as parameters and returns Z3 predicates. CertiQ offers a contract for all verified library functions and important types of potential user implementations. For implementations in CertiQ library, their contracts are statically verified; for user implementations like the BasicSwap pass, their contracts set the verification goals and define what it means by saying that the user code is verified. The purpose of contract-based design is twofold: first, it is for specifying the behavior of quantum data structures/operations that might be unexpected to classical world developers; more importantly, contracts provide a means to speed up symbolic **execution** through a mechanism that can be interpreted as predicate abstraction (see $\S4.2$).

Contracts for library functions. We give several simple examples of contracts used in our **BasicSwap** pass. More quantum-related contracts will be discussed in §4.3. For example, the contract of the Layout object is:

```
class Layout():
    ... # omitted code
    # Contract of the Layout object
    def precondition(self): return True
    def invariant(self): return True
    def postcondition(self):
        i = fresh_int()
        return ForAll([i], self.p2v(self.v2p(i))==i)
```

The non-trivial part of this contract is its post-condition, which specifies that both the two maps in Layout must be bijiections and the inverse of each other. For functions, their contracts are encoded in separate contract functions. For example, for the function simple_layout that generates an initial mapping of a circuit onto the coupling map of a physical device,

```
def simple_layout(qreg, coupling_map):
    layout = Layout()
    for i, qubit in enumerate(qreg):
        layout[qubit] = i
    return layout
```

its pre-condition function is,

which states that the inputs must comply with the post-condition of their classes and the size of the coupling map must be equal or larger than the size of the quantum register. Its post-condition function simply returns layout.postcondition. To prove the function simple_layout complies with its contracts, in CertiQ we verify the following,

```
# evaluate pre-condition
pre = simple_layout_pre(qreg, coupling_map)
# evaluate invariant before execution
inv_before = simple_layout_inv(qreg, coupling_map)
# symbolic execution
layout = simple_layout(qreg, coupling_map)
# evaluate post-condition
post = simple_layout_post(layout)
# evaluate invariant after execution
inv_after = simple_layout_inv(qreg, coupling_map)
# {pre-condition} Execution {post-condition}
certiq_prove(Implies(pre, post))
```

pre-condition => invariant
certiq_prove(Implies(pre, inv_before))
invariant before => invariant after
certiq_prove(Implies(inv_before, inv_after))

Another example is the function shortest_path in the CouplingMap class in the BasicSwap pass to find the shortest path of two physical qubits on the coupling map. Its pre-condition function returns And(p1 < self.size, p2 < self.size, self.postcondition) (here self is the coupling map). Its post-condition function returns:

This states that the two neighboring physical qubits on the path must have distance 1 and the two ends of the path are the two input physical qubits.

Contracts for BasicSwap pass CertiQ predefined contracts for all types of potential user implementations of transpiler passes. As shown in Fig.5, the annotation @swap in the first line informs CertiQ that this is a swap insertion pass. For swap insertion passes, we require the following three conditions are met:

• The pass must preserve semantics, *i.e.*, the input DAGCircuit and output DAGCircuit must perform the same functionality.

```
# It must preserve the semantics
def basic_swap_post1:
    return equiv(input_dag, output_dag)
```

where **equiv** (defined in §4) checks the equivalence of the input and output DAGCircuit.

• The output DAGCircuit of the pass must conform to the coupling map of the physical device.

```
# All 2-qubit gates must have their
# operands mapped next to each others
# in the coupling map
def basic_swap_post2:
    post_predicate = []
    i = fresh_int() # symbolic index of gates
    twoQgate = outputdag.twoQgates[i]
    q1 = twoQgate.op1
    q2 = twoQgate.op2
    post_predicate.append(i <= output_dag.
        twoQgate_count)
    post_predicate.append(ForAll([i],
            coupling_map.distance(q1, q2) ==1))
    return post_predicate
```

• The pass must terminate for all input circuits. Since termination is in general undecidable, we do not provide a contract function for it but require users to provide a variable to serve as a *program mono-tone*. A detailed example is given in §5.1.

Then, the verification goal of the BasicSwap pass in CertiQ is to symbolically prove that the above contracts functions.

3.4 Static analysis and code transformations

Before we hand over the **basic_swap** pass to the Z3 SMT solver, we statically analyze [33] its code and perform transformations to assist and speed up the symbolic execution. For example, the invocation of **simple_layout** will be replaced by its contract,

In this way, the symbolic execution does not need to unfold the implementation of simple_layout every time it is invoked. Then, the Z3 code and predicate generated by verifying BasicSwap will be in a tractable size and greatly reduce the burden of the SMT reasoning. As an example, with the predicate provided by shortest_path's contract that shortest_path the distance of succinct qubits are of distance 1, it is not hard for Z3 to prove the second verification goal that BasicSwap does output a DAGCircuit that conform to the coupling map of the physical device.

3.5 The visualizer

If there is a bug in the user code, the verifier will invoke the visualizer and generate a counter-example. If the verification cannot finish in a certain amount of time or there are unsupported external library calls in the submitted code, we exit with "undetermined."

3.6 The translation validator

If the BasicSwap pass cannot be verified automatically, *i.e.*, either the verification does not stop for a certain period of time or exits with "undetermined," CertiQ provides a translation validator at runtime. The algorithm of the translation validator is illustrated in detail in §4.4.

4 The CertiQ Framework

In this section, we discuss the two main technical contributions in CertiQ: the *calculus of quantum circuit equivalence* with the subsequent contract designs and *specification refinement* for quantum data structure verification. First, we define the equivalence of quantum circuits and how we use the calculus of quantum circuit equivalence to efficiently check the equivalence.

4.1 Equivalence checking for quantum circuits

The problem of equivalence checking of quantum circuits falls into the complexity class of QMA (the quantum version of NP) [21], thus it is intractable to verify the equivalence of quantum circuits by its denotational semantics. To enable the efficient equivalent checking for a large set of quantum circuits, CertiQ introduces the calculus of quantum circuits equivalence that is proven to be sound with respect to our denotational semantics of quantum circuits.

$$\begin{split} C &:= \operatorname{skip} & U &:= u_1(\lambda) \mid u_2(\phi, \lambda) \\ &\mid U(q_1, q_2, ..., q_n) & \mid u_3(\theta, \phi, \lambda) \\ &\mid C_1; \ C_2 & \mid X \mid Y \mid Z \mid H \\ &\mid CX \mid CY \mid CZ \\ &\mid \operatorname{SWAP} \mid \operatorname{measx} \mid \operatorname{measz} \end{split}$$

Fig. 6. Abstract syntax of quantum circuits in CertiQ. C are quantum circuits and U are unitary/non-unitary quantum operations. u_1, u_2, u_3 are physical 1-qubit gates that can be directly executed on IBM's machine, their definitions are given in Table 1 in §5.2.

Abstract syntax. Figure 6 shows the abstract syntax of quantum circuits in CertiQ. It shows that quantum circuits can be empty, unitary quantum gates, and combined sequence of quantum circuits. The equivalence of two quantum circuits C_1 and C_2 is then defined using the equality of their denotational semantics, $\forall nqreg : [C_1]_{nqreg} = [C_2]_{nqreg}.$

Denotational semantics. Denotational semantics of quantum circuits can be conveniently defined as their corresponding unitary matrices (Fig. 7).

Proving equality using denotational semantics, however, is exponentially hard since the dimension of matrices is $2^{nqreg} \times 2^{nqreg}$. To make the equality checking

$$[skip]_{nqreg} = I_{2^{nqreg}}$$

$$\llbracket U \rrbracket_{nqreg} = gate_def(U, q_1, ..., q_n, qreg)$$
$$\llbracket C_1 ; C_2 \rrbracket_{nqreg} = \llbracket C_1 \rrbracket_{nqreg} \times \llbracket C_2 \rrbracket_{nqreg}$$

Fig. 7. Denotational semantics of quantum circuits and unitary operations in CertiQ. nqreg is the number of qubits in the quantum registers used in the circuit. gate_def is a function in CertiQ that can evaluate the unitary matrices for quantum operations in the quantum register environment of qreg.

$$\frac{C_1 \equiv C}{C \equiv C} \text{ Symmetry } \frac{C_1 \equiv C_2}{C_2 \equiv C_1} \text{ Reflexivity}$$

$$\frac{C_1 \equiv C_2 \qquad C_2 \equiv C_3}{C_1 \equiv C_3} \text{ Transitivity}$$

$$\frac{C_1 \equiv C_2 \qquad C_1' \equiv C_2'}{C_1; C_2 \equiv C_1'; C_2'} \text{ Sequencing}$$

$$\frac{\text{equiv}(C_1, C_2)}{C_1 \equiv C_2} \text{ Primitive Patterns}$$

Fig. 8. The calculus of quantum circuit equivalence.

tractable, we design a calculus of quantum circuits equivalence by introducing a library of primitive patterns of circuit equivalence.

The calculus of quantum circuits equivalence. Figure 8 shows the inference rules of our calculus of quantum circuits equivalence, including the rules of symmetry, reflexivity, transitivity, and sequencing. All the rules are straightforward except for the rule of primitive patterns. CertiQ introduces a predicate equiv specifying a set of primitive patterns of circuit equivalence (see Fig. 9). For example, equiv([CNOT(q_1, q_2), Z(q_1)], [Z(q_1), CNOT(q_1, q_2)])gives us the commutativity rule between the CNOT and the Z gate. These primitive patterns are small enough to be verifiable by calculating their denotational semantics in CertiQ. For example, the second cancellation rule in Fig. 9 can be proven as follows,

$$\begin{bmatrix} \mathbb{H} \end{bmatrix} \cdot \begin{bmatrix} \mathbb{H} \end{bmatrix} = \frac{\sqrt{2}}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \cdot \frac{\sqrt{2}}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$
$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \text{(Identity)}$$

With proved primitive circuit patterns, we proved that our calculus of quantum circuit equivalence is sound.

Theorem 4.1 (Soundness).

$$\forall C_1 \ C_2 \ nqreg, \ C_1 \equiv C_2 \ \Rightarrow \ [C_1]_{nqreg} = [C_2]_{nqreg}$$



Fig. 9. Examples of certified primitive patterns implemented by equiv in CertiQ. They are bridging rules (above), cancellation rules (2nd line), commutativity rules (3rd, 4th line), and swap rules (bottom).

Experiments (see §6) shows that this calculus of circuit equivalence is able to decouple the underlying quantum complexity from the verification and enables efficient automated reasoning in the symbolic execution.

On the other hand, the certified primitive patterns defined in Fig. 9 are also implemented as library functions and served as atomic circuit transformations in transpiler passes. Comparing to allowing developers arbitrarily modify quantum circuits, this design is advantageous in terms of code quality management and facilitation of symbolic reasoning. For example, the last swap rule in Fig. 9 defines the swap_and_update_layout primitive we used in BasicSwap pass, which first inserts a swap gate and then updates the layout. Since the BasicSwap pass changes circuits only through this atomic swap_and_update_layout primitive, which has been proven to preserve semantics, **BasicSwap** can be trivially verified. In contrast, before CertiQ, the implementation of BasicSwap pass in Qiskit performed swap insertion and layout update in separate loops, breaking the equivalence of intermediate circuits in the between two loops, making the symbolic verification much harder:

```
# Previous implementation of BasicSwap in Qiskit
for layer in dag.serial_layers():
    subdag = layer['graph']
    for gate in subdag.twoQ_gates():
        ... # Other codes
        # create the swap operation
        for swap in range(len(path) -2):
            swap_layer.apply_operation_back(SwapGate(),
```

args=[q1, q2],cargs=[])

As shown in the code above, the circuit transformations used do not preserve semantics all the time, thus no well-behaved contract can be given to these functions. More importantly, this original implementation cannot be verified automatically since loop invariants cannot be given for the variable-length loops in the code. Next, we discuss the use of contracts in loop invariants search as well as in general symbolic execution.

4.2 Contracts for scaling symbolic execution

Contracts enables the modular verification in CertiQ. Consider the general case in a symbolic execution,

... # execution
qiskit_call(para)
... # continue execution

where $qiskit_call$ is a Qiskit Terra library function, with the call parameter *para*, pre-condition *pre(para)*, and post-condition *post(para)*. CertiQ enables the predicate abstraction, meaning that we can use the contract of a function without symbolically executing that function. Take the invocation of $qiskit_call$ (that has been verified to satisfy its contracts) as an example. Suppose the program state before the invocation is specified by the Z3 predicate *s*. To invoke this primitive, the precondition in the contract has to be satisfied, *i.e.*, $s \Rightarrow pre(para)$. With predicate abstraction, instead of performing the symbolic execution of the function body, the predicate after the invocation is:

$$s \wedge post(para)$$

This significantly reduces the burden of the symbolic reasoning.

Contracts for user functions. CertiQ provides several pre-defined contracts that users can apply to their functions, some of which can be automatically inferred. For example, if a function returns a layout, CertiQ will automatically add the bijection requirement for the returned layout. Some of the pre-defined contracts have to be hinted at by users. For example, if users provide the annotation "@coupling_map_path" at the beginning of a function, the CertiQ verification engine will apply the corresponding contract. Thus, the post-condition of a coupling map is applied, which is that the distance between the *i*th element and i + 1th element of the returned path must be 1 on the input coupling map.



Fig. 10. Quantum data structures of qubit states (top) and quantum gates (bottom). These data structures are used for optimizing 1-qubit gates. State vector and unitary matrices representation serves as the specifications for these data structures. After performing the refinement test, we show that Bloch sphere is not equivalent to state vector representation and unit Quaternion presentation in multi-qubit cases, because they lost the global phase information. For quantum gates, unit Quaternion representation and Bloch sphere representation are not equivalent to unitary matrices.

Loop invariants. The SMT backend cannot handle variablelength loops, thus loop invariants must be inferred or provided in CertiQ for successful automated verification. Fortunately, in this domain-specific environment (a quantum compiler), practically, this problem can be more easily solved than in the general case: loop invariants might be found with heuristics leveraging the domain knowledge provided by the contracts in the loop body. In CertiQ, we use the simple heuristics that test if the contracts of the library functions invoked in the loop body are loop invariants. With the use of certified library functions (whose contracts usually provides the loop invariants), this heuristics works well in practice for verifying transpiler implementations.

If loop invariants for a loop cannot be found by CertiQ, the user can choose to provide the invariant using annotations.

4.3 Specification refinement for equivalence of quantum data structures

As a quantum software, Qiskit has a rich variety of quantum data structures that represent the underlying quantum objects. For example, as discussed in §2, there are three data structures for quantum circuits: Quantum-Circuit and DAGCircuits as well as the abstract circuit in CertiQ. There are also three data structures for qubit states, *i.e.*, state vector representation, Bloch sphere representation and unit Quaternion representation (Fig. 10



Fig. 11. The simulation diagram for refinement saying that, starting from a pair of equivalent concrete DAG D_C and abstract DAG D_a , for any transformation t, if t transforms D_C to D'_C , then t must transform D_a to an abstract DAG D'_a that is equivalent to D'_c .

top) and quantum gates (Fig. 10 bottom). In CertiQ, we statically verify the equivalence of these quantum data structures. Take the DAGCircuit and QuantumCircuit as an example, the refinement requirement can be informally stated as: if we feed a pair of equivalent DAG-Circuit and QuantumCircuit into a function performs circuit transformation, it should yield another DAGCircuit and another QuantumCircuit which are equivalent to each other. Thus any transformations cannot break the equivalence. More precisely, in CertiQ, for each pair of equivalent quantum data structures, we define the equivalence relation " \cong " between them. For example, for a DAGCircuit D_c and a QuantumCircuit Q_c , CertiQ defines \cong to be,

$$D_c \cong Q_c \iff \forall i, D_c.topological_op_node(i) = Q_c(i)$$

where topological_op_node will return a list of gates in the DAG sorted by their dependence. Then the refinement property can be formally defined in a simulation diagram [24] in Fig. 11. In CertiQ, we prove the refinement property for equivalent data structures by symbolic execution in Z3 solver and found that between several important data structures that represents qubit space, the refinement property breaks.

An example: Bloch sphere representation. The Bloch sphere representation [4] is a commonly used data structure for qubit states, in which the logical state $|0\rangle$ is mapped to the north pole and $|0\rangle$ is mapped to the



Fig. 12. The Bloch Sphere represents a single qubit. The $|0\rangle$ state is on the North Pole, the $|1\rangle$ state is on the South pole, and superposition states are in between. Single qubit gates correspond to rotations on the Bloch sphere. For instance, the Z gate rotates a qubit by angle π about the Z-axis. south pole (see Fig. 12). Specifically, Bloch sphere representation is a projection where the global phase of a qubit state $|\psi\rangle$ is omitted and $|\psi\rangle$ and $e^{i\gamma} |\psi\rangle$ are mapped to the same qubit state. The main part of this projection can be seen trivially in the following Python code,

def Bloch_rep(gamma, theta, phi):return (theta, phi)

where a general qubit state ψ ,

$$|\psi\rangle = e^{i\gamma}\cos(\frac{\theta}{2})|0\rangle + e^{i(\phi+\gamma)}\sin(\frac{\theta}{2})|1\rangle)$$

parameterized by (γ, θ, ϕ) is projected to the spherical coordinate (θ, ϕ) of a unit sphere. Between state vector representation (which we view as the specification) and Bloch representation, the equivalence relation " \cong " is defined by the above Bloch_rep function. However, the refinement property does not hold for it, since there is a transformation tensor_product together with other multi-qubit operations that breaks the diagram in Fig. 11. Refinement breaks because there is an untracked phase difference between qubits beyond the 1-qubit case. The relative phase change will induce non-trivial quantum computation that is not revealed in this representation. To address this issue, in CertiQ we explicitly exclude any multi-gubit operations in the contract of any transformations conducted in the Bloch sphere representation. This restriction also applies to the unit quarternion representation which proved to be equivalent to the Bloch sphere representation. We will use these conclusion in the experiment in $\S5.2$.

4.4 The translation validator



Fig. 13. Translation validation of swap insertion passes. (a) and (b) show the input circuit and the output circuit of the swap pass. First, the validator performs a swap_and_update_gate (the dashed-line box in (c)) behind every swap in (b), which is a primitive circuit move. Then the validator performs the primitive circuit move cancel_swap (the dashed-line box in (d)). Then we recover the input circuit.

For two important types of transpiler passes, CNOT optimization passes and swap insertion passes, that receives the most community contributions, CertiQ also

provides a translation validator if the symbolic verification of a pass fails. The translation validator verifies the equivalence between a specific input and its output from the transpiler pass to be verified. This is done by reverting the changes of the pass it validates. As an example, we illustrate the validation algorithm of swap insertion passes with an input circuit of 3 qubits in Fig. 13. We assume the coupling map for the three qubits is $q_1 - q_2 - q_3$. For validating swap passes with the intput in Fig. 13(a), the validator finds swap gates in the mapped circuit and insert another swap gate right behind each with the swap_and_update_gate method (which is semantics preserving). After all swaps getting cancelled out by applying the cancel_swap method, we recover the input circuit. For validating the output of CNOT cancellation pass, a similar algorithm is performed.

5 Case studies

Here we present case studies to show how CertiQ detects bugs and safety issues in realistic settings. We find a counter-example circuit that the lookahead_swap pass does not terminate on, we point out a bug in the optimize_lq_gate pass that can be addressed by specifying correct contracts for the pass and the function calls inside, and we identify two bugs in the commutative_analysis and commutative_cancellation passes when specifying their contracts.

5.1 swap insertion passes

Swap insertion passes are a fundamental stage of compiling for NISQ machines, where qubits are not fully connected and must be swapped on a chip to communicate. Because swap gates are error-prone and can corrupt the whole computation, these passes try to minimize the number of swap operations.

In the case study described here, we show how CertiQ identify a bug in the lookahead_swap pass.

As mentioned in §3, there are three verification goals for swap passes: (1) the pass must be semantics preserving; (2) The output DAGCircuit of the pass must conform to the coupling map of the physical device; (3)The pass must terminate. Proving the first two goals is demonstrated in §3. For the third verification goal, CertiQ does not try to solve it completely because it is undecidable. Instead, CertiQ aims to provide sound termination analysis for practical implementations. First, CertiQ concretizes the problem to verify the termination of passes with input circuit of bounded depth on a given coupling map. Termination can be proved by constructing strictly monotonic functions in a finite domain. For program states that are not in a loop or a recursive function, the program counter is a monotonic function to provide termination guarantee. For variable-length

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loops and while loops, CertiQ allows users to provide the monotonic function, for example,

```
gates_remaining = dag.topological_op_node()
while gates_remaining != 0:
# @mono: -gates_remaining.size
... # implementation code
```

Then in the backend SMT solver, the verifier solves for the circuit input that keeps gates_remaining.size unchanged and gives it as a counter example.

We verified three swap insertion passes: basic_swap, lookahead_swap and noise_adaptive_swap. We report that all three passes comply with the first two contracts. However, we find a counter-example circuit on coupling map of the IBM 16 qubit device, where the lookahead_swap pass does not terminate on (see Fig. 14). The lookahead_swap pass greedily finds the next best 4 swap gates to minimize the totl distance of the unmapped 2-qubit gates. However, the counter example we found shows that the 4 swap gates can cancel each other out with the swap rules in Fig. 9, thus gate_remaining.size will not update.

5.2 The optimize_1q_gate pass

We next focus on the verification of the optimize_lq_gate pass and show that, with contract-based design, we can reveal bugs only arise in quantum software.

We verify the re-implemented optimize_1q_gate pass using the merge_1q_gate method. This pass collapses a chain of single-qubit gates into a single, more efficient gate [42], to mitigate noise accumulation. It operates on u_1, u_2, u_3 gates, which are native gates in the IBM devices. These gates can be naturally describe as linear operations on the Bloch sphere, for example, u_1 gates are rotations with respect to the Z axis. For clarity, we list their matrix representations in Table 1.

$$u_1(\lambda) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\lambda} \end{pmatrix}, \quad u_2(\phi, \lambda) = \frac{\sqrt{2}}{2} \begin{pmatrix} 1 & -e^{i\lambda} \\ e^{i\phi} & e^{i(\lambda+\phi)} \end{pmatrix}$$
$$u_3(\theta, \phi, \lambda) = \frac{\sqrt{2}}{2} \begin{pmatrix} \cos(\theta) & -e^{i\lambda}\sin(\theta) \\ e^{i\phi}\sin(\theta) & e^{i(\lambda+\phi)}\cos(\theta) \end{pmatrix}$$

Tab. 1. Matrix representation of physical gates u_1 , u_2 and u_3 . u_1 is a Z rotation on the Bloch sphere.



Fig. 14. (left) A counter-example generated by CertiQ that shows Qiskit's lookahead_swap pass does not always terminate on the IBM 16 qubit device. (right) The coupling map of the IBM 16 qubits device. Arrows indicate available CNOT directions (which does not affect the swap insertion step).

The optimize_lq_gate pass has two function calls. First, it calls the collect_runs method to collect groups of consecutive u_1 , u_2 , u_3 gates. Then it calls merge_lq_gate to merge the gates in each group. merge_lq_gate (Fig. 15) first transforms the single qubit gates from the Bloch sphere representation to the unit quaternion representation [18], then the rotation merges are performed in that representation.

As described in §4.3, the contracts of these two representations allow only single-qubit operations required by the refinement property. However, every Qiskit gate can be modified with a c_if or q_if method to condition its execution on the state of other classical or quantum bits. When the transpiler pass attempts to optimize these conditional gates, it can lead to a wrong circuit. For this reason, in the contract and implementation of collect_runs, we have to include that gate1.q_if == False and gate1.c_if == False.

The bugs described above, which relate to how quantum circuit instructions can be conditioned, have been observed in Qiskit in the past [35, 36]. In the absence of rigorous verification like this work, such bugs are hard to discover. In practice, this is usually done via extensive randomized testing of input/output circuits, which does not provide any guarantee. The results demonstrate that our contract for merge_1q_gate based on contextual refinement is effective for detecting quantum-related bugs.



Fig. 15. Correct execution (top) and incorrect execution (bottom) of merge_lq_gate.

5.3 commutation passes

commutation_analysis and commutative_cancellation is a pair of Transpiler passes that optimizes DAGCircuits using the quantum commutation rules and the cancellation rules in Fig. 9. First, commutation_analysis transforms the DAGCircuit to a representation called commutation groups [43], where nearby gates that commute with each other are grouped together. Then commutative _cancellation performs cancellation inside groups. In Fig. 16, we give a working example.

We find two bugs when verifying this pair of passes. First, the commutation group can be viewed as an abstract specification for the DAGCircuit. However, when specifying the contract of commutation_analysis, we find



Fig. 16. A working example of commutation_analysis and commutative_cancellation. (a) the un-optimized circuit; (b) commutation_analysis forms the commutation group (c) commutative_cancellation cancels self-inverse gate inside groups.

that the commutation group representation violates contextual refinement property defined in §4.3. This violation comes from the fact that the commutation relation is in general not transitive. For example, if we denote the commutation relation as ~ and there are 3 quantum gates, A, B, C, where A ~ B, B ~ C, then A ~ C is not guaranteed to be true. For this reason, gates with pairwise commutation relation cannot be grouped together. We propose two solutions to this bug. First, we can make sure the circuits that these passes operate on have a limited gate set where ~ is indeed transitive. For example, in the gate set {CNOT, X, Z, H, T, u_1, u_2, u_3 }, ~ is transitive. Second, we can use a new algorithm that does not assume transitivity but is potentially less efficient.

The second bug we find is when specifying the contract of commutative_cancellation. The bug is the same to the bug in §5.2, where the pass cancels gates with a classical control. This bug can be fixed by asserting that gate.c_if==False and gate.g_if==False.

6 Evaluation

We performed verification of four transpiler phases with seven implementations. The seven implementations are: the collect_2q_block pass, the commutative_analysis pass, the commutative_cancellation pass, the lookahead _swap pass, the basic_swap pass, the noise_adaptive_swap pass, the optimize_1q_gate pass. These passes are all re implemented with invariant-guided contract design. With seven successful verifications (none exit with "undetermined"), we report three bugs. We evaluate CertiQ based on the verification of these implementations.

Verification performance For implementations using our certified circuit patterns, all transpiler passes can be verified within seconds. However, most of the original implementations cannot be verified or take long time to verify.

Run-time performance. When executing, verified code still calls functions from the Terra library, not from the specifications in CertiQ, so its performance is not affected. However, the interface of primitive circuit moves

indeed adds some constraints on the allowed operations. For example, when using the swap_and_update_gate method in a loop to swap along a path, the complexity is $O(n^2)$, where n is the number of gates in the circuit. While using the swap method in a loop to achieve the same is of complexity O(n). We mitigate this problem by verifying the efficient implementation and providing it as a primitive move. For example, in CertiQ we verify the above implementation with the swap and provide it as the swap_along_path method.

Extensibility. The contract-based design provides a powerful abstraction for complicated optimization algorithms, thus we believe CertiQ is extensible to future transpiler implementations. On the other hand, since CeritQ already provides abstract specifications and contracts for important data structures in Qiskit, we expect CertiQ to be very extensible for other components of the Qiskit toolchain that rely on the same infrastructure.

7 Related work

Quantum programming environments with a verifier. Several quantum programming environments support the verification of quantum programs running on it. For example, in the QWire quantum language [38, 40], programmers can use the embedded verifier based on the Coq proof assistant [7] to perform mechanized proof for their programs. The $Q |SI\rangle$ programming environment [26] allows users to reason about their programs written in the quantum **while**-language with quantum Floyd-Hoare logic [51]. In contrast to CertiQ, these environments require expertise both in quantum computing and formal verification to construct proofs and these proofs verify at the program level, not the compilation level.

Verified quantum-related compilers. Previous studies on compiler verification for reversible circuits [3], ancillae uncomputation [38, 39] and compiler optimizations [19] utilize interactive theorem provers such as F^* [29] and Coq [7] to conduct manual proofs, which do not provide an extensible interface for developers to verify future extensions with low proof burden. In contrast, CertiQ verification framework allows developers to plugin their implementations that can be verified in a mostly-automated manner.

Algorithms to perform efficient quantum circuits equivalence checking have been discussed from the view of quantum algorithms [49], quantum communication protocols [5], and verification of compilation [2]. However, while powerful, these checking algorithms are too complicated to automated verification like we use with CeritQ. Model checking in quantum computation verification. The early adoption of Model checking in quantum computation focused on verifying quantum communication protocols [10, 17, 47, 52]. Recently, model checking techniques have been applied to more areas, including quantum Markov chain analysis [13–15], checking physical systems, program analysis [22, 25, 53]. However no automated verification tool based on model checking like CertiQ exists for quantum computing until now.

Push-button verification in classical computing. Pushbutton verification has been applied for building verified file systems, OS kernels, and system monitors [30, 31, 44]. Our technical choice and many of the verification ideas are heavily influenced by these previous work. However, these systems cannot support variable-length loops, calculus of quantum circuit equivalence, and our contractbased reasoning.

8 Conclusion and Future Work

We presented CertiQ, a mostly-automated verification framework for the Qiskit compiler that addresses the key challenges of verifying a real-world quantum compiler. CeritQ introduces the calculus of quantum circuits equivalence to statically and efficiently reason about the correctness of compiler transformations. CertiQ introduces a combination of proof techniques to reduce verification complexity from the underlying quantum computation as well as from the large user code space. These proof techniques include SMT reasoning, contractbased design, and invariant contract. With extensive case studies, we demonstrate that CertiQ can detect critical bugs, some of which are unique to quantum software.

To our knowledge, CertiQ is the first effort enabling the automated verification of a real-world commercial quantum compiler. The approach we establish with CertiQ paves the way for end-to-end verification of a complete quantum software toolchain, an important step towards practical near-term quantum computing. Going forward, we are working to use our contract-based approach to incorporate verification of both higher and lower components of Qiskit. These include Qiskit Aqua, the high-level quantum algorithm library and the OpenPulse interface [28], which implements quantum operations through microwave control pulses.

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