Contract-based verification of a realistic quantum compiler

Yunong Shi*
The University of Chicago yunong@uchicago.edu
Xupeng Li*
Columbia University xupeng.li@columbia.edu
Runzhou Tao
Columbia University runzhou.tao@columbia.edu
Ali Javadi-Abhari
IBM T.J. Watson Research center Ali.Javadi@ibm.com
Andrew W. Cross
IBM T.J. Watson Research center awcross@us.ibm.com
Frederic T. Chong
The University of Chicago chong@cs.uchicago.edu
Ronghui Gu
Columbia University ronghui.gu@columbia.edu

ABSTRACT
In this paper, we present CertiQ, a mostly-automated verification framework for the Qiskit quantum compiler. To our knowledge, CertiQ is the first effort to apply formal verification and SMT reasoning to a real-world quantum compiler. Qiskit is currently the most complete and 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 (called Terra), providing abstract specifications for quantum compiler data structures and offering verifiable contracts that specify the behaviors of compilation phases with heavy optimizations. CertiQ enables verification of existing implementation of the Qiskit compiler and future code submissions in a mostly-automated manner using invariant-guided contracts and contract continuation. 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 [29] (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, 31].

Qiskit [1] is currently the most complete and widely-used open-source software stack. Qiskit lets users design and run quantum programs on the IBM Q cloud [19], 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 open-source community: with 180k downloads, 1500 Github forks (with 2nd place Cirq [6] < 500) and Github "usedby" of 122 (with 2nd place Qutip [34] 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 [41]; demonstration of error detection schemes [46]; demonstration of quantum machine learning algorithms [38, 50].

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 [44] related to the compilation process highlights the crucial need for effective, reliable and automated methods to verify near-term quantum computations down to the compilation level.

*Both authors contributed equally to this research.
We introduce CertiQ, a mostly-automated verification framework for Qiskit Terra. To our knowledge, CertiQ is the first effort to apply formal verification and SMT reasoning to real-world quantum compiler. The design philosophy underpinning CertiQ is motivated by three practical challenges that arise when providing correctness guarantee to Qiskit Terra.

The first challenge is that checking the equivalence of quantum circuits is generally intractable [20]. To mitigate this problem, in CertiQ we define a verifiable small-step operational semantics for quantum circuits that we call primitive circuit moves that circuit equivalence and the correctness of compiler transformation can be efficiently proved. Our semantics is proven to be sound and therefore faithful to the underlying quantum computation.

The second challenge for correctness guarantee 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. Using the Design-by-Contract methodology, CertiQ offers contracts to specify the behaviors of quantum data structures and library functions in Qiskit Terra, for example, the Bloch sphere representation of qubit states. With the contract-based design, we are able to reason about the invocation of a verified function using its contract without looking into its concrete implementation. We design, specify, and verify a library of functions that perform primitive circuit transformations with invariant-guided contracts. Compilation phases implemented using this library can be easily verified. The reason is that these function calls can be treated as “transparent” in symbolic execution because their contracts imply semantics-preserving.

The third challenge is that compiler implementations in future code submission can be very complicated, making mostly-automated verification hard. By “mostly-automated”, we mean that programmers have to write little to no annotations to assist the verification. To achieve this level of automation, CertiQ first pre-processes code by replacing its calls to library functions with their abstract specifications and contracts. CertiQ 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]. CertiQ introduces contract continuation to automatically infer the contracts of developers (contributors) defined functions and simplify contracts in verification. CertiQ also provides several types of commonly used contracts for developers to specify their functions. Further, with careful design of function calls and their contracts, the effect of CertiQ verification on compilation performance is not noticeable.

For several 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 small overhead. The translational validator itself is also verified.

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 provide small-step semantics for quantum circuit equivalence and formal specifications of quantum circuit transformations that efficiently prove compiler optimizations are semantics preserving.
- We introduce a contract-based design that specifies the behavior of other operations, thereby facilitating modular verification of quantum compiler implementations.
- We build a transformation library verified with respect to its contract, which guarantees that the provided circuit moves preserve the circuit equivalence. This library can be used to build verified quantum compilers.
- We combine proof techniques including static analysis, SMT theory reasoning, and contract continuation that make CertiQ scalable and mostly-automated.
- We verify a series of Qiskit Terra optimizations and discover five critical bugs. Some of these bugs are unique to quantum software.

The paper is organized as follows: section 2 introduces background on quantum computing and Qiskit Terra; section 3 provides an overview of the CertiQ framework; section 4 discusses technical contributions of CertiQ; section 5 presents case studies demonstrating how CertiQ works in the realistic settings; section 6 evaluates the correctness and performance; section 7 discusses previous works; section 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 $|0\rangle$ and $|1\rangle$. The general quantum state of a qubit is represented as $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$ (or in its vector form $\alpha, \beta$), where $\alpha, \beta$ are complex coefficients with $|\alpha|^2 + |\beta|^2 = 1$. When
This property sets the foundation of quantum speedup circuit. Executed by introducing quantum SWAP gates into the constraints of the QIP platform. This process is usually composed quantum circuit conforms to the topological detection [40].

Rewriting [42], template matching [26], commutativity involves post-decomposition optimizations like circuit computation and communication.

The circuit for preparing the 3-qubit GHZ state SWAP gate to 3 alternating CNOTs; decomposition of examples of circuit decomposition: decomposition of a into quantum circuits. Figure 1 illustrates two simple

![Image of circuit](image1)

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).

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 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 high-level description of quantum algorithms to a circuit consisting of a series of quantum gates. A quantum 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 $|\psi_{\text{GHZ}}\rangle = \frac{1}{\sqrt{2}} (|000\rangle + |111\rangle)$, a quantum state used widely in quantum computation and communication.

The system-independent optimization stage (stage 2) involves post-decomposition optimizations like circuit rewriting [42], template matching [26], commutativity detection [40].

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 and pulses, optimizing 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. 3), 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. It stores the edges of the qubits in a list. For example, $\text{coup} = [[0,1],[1,2],[2,3]]$ 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,

```python
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 [22]. 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
This section gives an overview of the CertiQ framework by walking through the verification of a simple but less quantum-related transpiler pass. The integration of CertiQ and Qiskit Terra as a quantum software will be addressed in §4. 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. We use a simple transpiler pass named basic_swap as a running example to introduce the CertiQ verification workflow (see fig. 4).

3.1 Specifications
Specifications in CertiQ can be viewed as alternative implementations of quantum data structures and library functions in Qiskit Terra. They share the same interface with the original implementation but are re-implemented to support symbolic execution. Thus, we can verify contributors’ code by replacing the data structure operations and invocation of Terra library functions with CertiQ specifications, and then feed the specifications into our verification engine. There are two kinds of specifications: trusted specifications and abstract specifications.
 Trusted specifications. When replacing basic Python data structures with the ones in the SMT solver, e.g., Z3, the equivalence of the transformation is in our trusted computing base (TCB). These specifications are called trusted specifications. For example, the specification of the Layout data structure in CertiQ is

```python
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 with the only difference that Layout specification uses Z3 Map rather than Python dict. Here, we trust that Map in Z3 correctly specifies dict in Python.

 Abstract specifications. CertiQ allows users to lift some library implementations into abstract specifications to speed up the verification. For example, the abstract specification of the DAGCircuit class is an array of gates,

```python
class DAGCircuit: # dagcircuit specification
def __init__(self, gates=Array(IntSort(), GateType)
    if gates is None else gates)

The equivalence between all abstract specifications and their implementations is verified using contextual refinement (see §4.2).

 3.2 Contracts

The concept of contract is deeply rooted in the design of CertiQ, primarily for specifying the behavior of quantum data structures/operations that might be unexpected in classical software. CertiQ offers contracts for every object and method that their specifications must comply with. In CertiQ, a contract consists of three parts: pre-conditions, post-conditions, and invariants. We give several simple examples of contracts that will be used in our basic_swap pass. More quantum-related contracts will be discussed in §4.2. For example, the contract of the Layout object is

```python
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 bijections 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,

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

its pre-condition function is,

```python
def simple_layout.pre(qreg, coupling_map):
    return And(coupling_map.postcondition,
               qreg.postcondition,
               coupling_map.size == qreg.size)
```

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

```python
# 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 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

```python
And(ForAll([i],
    Implies(And(i ==0, i < self.size - 1),
    self.distance( self.shortest_path[i],
                  self.shortest_path[i+1]) == 1)),
    self.shortest_path[0] == p1,
    self.shortest_path[1] == p2)
```

Which states 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.

The basic_swap pass. With the previous function definitions and their contracts, we can look into the implementation of the basic_swap pass (see fig. 5). This pass brings the qubit operands together for every 2-qubit gate in a DAGCircuit so that the 2-qubit gate operations can be done in two connected qubit locations on
# @swap
class BasicSwap(TransformationPass):
    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.qreg, 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 basic_swap pass.

the coupling map. The implementation invokes a function swap_and_update_gate(i,j) to insert quantum gate swap(i,j). In §4, we will see it is an invariant-guided contract design, whose invariant is equiv(input_dag, output_dag), stating that the DAGCircuits before and after inserting swap are equivalent.

In Fig.5, comment # @swap in the first line is a developer annotation informing CertiQ that this is a swap pass such that the CertiQ engine can automatically generate its corresponding contract as below,

```python
# It should preserve the semantics
def basic_swap_inv:
    return equiv(input_dag, output_dag)
```

which is the same with the invariant of the swap_and_update_gate method. For simplicity, here we just list the invariant, we will discuss other parts of its contract in §5.1.

### 3.3 The verification goal

The verification goal of the CertiQ engine is to prove that every function call in the submitted code complies with its contract. For example, when our basic_swap pass is submitted for code review, the verification engine will prove that the basic_swap pass and (specifications of) all the functions called by it comply with their contracts if they possess one. Any calls to the Qiskit library will be directed to their abstract specifications. CertiQ has already verified these library calls with respect to their contracts.

### 3.4 Static analysis and code transformations

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

```python
# Check pre-condition
certiq_prove(simple_layout_pre(dag.qreg, self.coupling_map))
# Impose post-condition
simple_layout_post(layout)
```

In this way, the symbolic execution does not need to unfold the implementation of simple_layout every time it is invoked.

Another powerful transformation that can further reduce the verification complexity is called contract continuation. Intuitively, if a function does nothing but calls another function in its function body, then the contract of the callee can be continued to the caller function if the caller does not have a contract. This applies to the for loops in the example of basic_swap. Since the inner loop only has one child swap_and_update_gate, thus, the invariant in its contract continues to the loop function. In CertiQ, the static analyzer progressively propagates the contract and tests if the contract holds. Then, by this continuation, the basic_swap pass have the invariant of swap_and_update_gate propagated to it, which validates its contract and finish the proof.

### 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

For two important types of transpiler passes, swap insertion passes and CNOT gate optimization passes, if CertiQ cannot verify the code (either verification does not stop for a certain period of time or exits with “undetermined”), a translation validator will be invoked to validate the compilation results at runtime. The translation validator itself is verified by the CertiQ verification engine.

### 4 THE CERTIQ FRAMEWORK

In this section, we discuss the main technical contributions in CertiQ and how they are integrated into Qiskit as a quantum verification framework. Most of the proof techniques we introduce are for the purpose of reducing
the verification complexity, either of the underlying quantum computation or of potential state explosion from future code submission. We start a description of the formal semantics of quantum circuits defined in CertiQ, with which can be verified efficiently if a transformation is semantic preserving. We then discuss specifications for quantum data structures followed by the introduction of the invariant-guided contract design for library functions and contract continuation for user defined functions.

4.1 Primitive circuit moves

The problem of equivalence checking of quantum circuits falls into the complexity class of QMA (the quantum version of NP) [20], thus it is intractable to verify the equivalence of quantum circuits in their denotational semantics (unitary matrices). For efficient verification, in CertiQ we define small step operational semantics for DAGCircuits (quantum circuits). We call these small step semantics primitive circuit moves. These moves are implemented in CertiQ by the functionequiv:DAG→DAG→Boolean. The input and output of primitive circuit moves are evaluated to be True by equiv. For example, equiv([\text{CNOT}(q_1, q_2), Z(q_1)], [Z(q_1), \text{CNOT}(q_1, q_2)]) = True gives us the commutativity rule between the CNOT and the Z gate (see fig. 6). We still define the denotational semantics of quantum gates to be their unitary matrices so that the soundness of primitive circuit moves can be proved by direct simulation. Thus we can say that the equivalence relations we define are faithful to the underlying quantum computation. In this way, we define formal semantics that allow us to conduct efficient verification.

4.2 Specification refinement

We say a specification and an implementation are equivalent if they satisfy the refinement property. Continuing with the example of DAGCircuit in §3, we describe how the equivalence of abstract specifications and implementation is proved in CertiQ. The refinement for DAGCircuit can be informally stated as: any transformation performed on a pair of equivalent abstract DAG (in specification) and concrete DAG (in implementation) should yield another pair of equivalent abstract DAG and concrete DAG. More precisely, in CertiQ we define the equivalence relation ~ between a concrete DAG \( D_c \) and an abstract DAG \( D_a \) as,

\[
D_c \sim D_a \iff \forall i. D_c.\text{topological\_op\_nodei} = D_a i
\]

where topological\_op\_node will return a list of gates in the DAG sorted by their dependence. Notice that ~ is defined differently from equiv since that ~ is a relation between abstract DAGs and concrete DAGs. With ~ defined, if we perform any transformation, for example appending a gate, on \( D_c \) and \( D_a \) where \( D_c \sim D_a \), then it must yield \( D'_c \) and \( D'_a \) respectively, where \( D'_c \sim D'_a \) as well. This property can be illustrated by a simulation diagram [23] in Fig. 7.

In CertiQ, we prove the refinement property for DAGCircuit by symbolic execution in Z3 solver, thus proving the equivalence between the abstract specification and the real implementation.

Bloch sphere representation. Bloch sphere representation [4] gives us an example of how contextual refinement can be used to specify the behavior of quantum objects. The Bloch sphere representation can be viewed as an abstract specification of the qubit states, in which \(|0\rangle\) is mapped to the north pole (see fig. 8). 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
We describe how contracts in CertiQ assist the symbolic execution. We explicit exclude any multi-qubit operations in the general case in symbolic execution, functions for which we cannot pre-define contracts. We also discuss user functions and show how contract design further reduces the complexity of symbolic execution in verification and how invariant-guided contracts.

Fig. 8. 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 \(\pi\) about the Z-axis. of this projection can be seen trivially in the following Python code,

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

where a general qubit state \(|\psi\rangle = e^{i\gamma} \cos\theta |0\rangle + e^{i\phi} \sin\theta |1\rangle\) parameterized by \(\gamma, \theta, \phi\) is projected to the spherical coordinate \(\theta, \phi\) of a unit sphere. The Bloch sphere representation can be seen as an abstract specification of qubit states, where the equivalence relation \(\sim\) is defined by the above `Bloch_rep` function. However, the contextual 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. 7. Contextual 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-qubit operations in the contract of any transformations conducted in the Bloch sphere representation. This restriction also applies to other qubit state representation in Qiskit Terra, for example the unit quaternion representation that will be discussed in §5.2.

### 4.3 Invariant-guided contracts

We describe how contracts in CertiQ assist the symbolic execution in verification and how invariant-guided contract design further reduces the complexity of symbolic execution. We also discuss user functions and show how to perform contract continuation and for user defined functions for which we cannot pre-define contracts.

Contracts in symbolic execution. We consider the general case in symbolic execution,

```python
...  # execution
terra_call(para)
...  # continue execution
```

where `terra_call` is a Qiskit Terra library function, with call parameter `para`, pre-condition `pre(para)`, post-condition `post(para)`. As shown in §3, the contract is also parameterized by `para` (we leave out the invariant for now). We denote the program state before entering `terra_call` as `s`, then `para` also depends on `s`. If the program is correct, we have \(s \Rightarrow pre(\text{para}(s))\). By Modus ponens and `s`, we have `post(\text{para}(s))`. Instead of continuing the symbolic execution inside the call, we directly conclude that the current program state is

\[
s \land post(\text{para}(s))
\]

This execution can be accomplished because CertiQ pre-verifies the contract of library function `terra_call`.

Our approach of applying contracts to symbolic execution can be viewed as fine-grained predicate abstraction \([8, 15]\) that minimizes the possibility of spurious counter-examples and greatly reduces verification complexity.

Invariant-guided contracts. If we assume further that `terra_call` is called in a loop,

```python
...  # execution
for i in range(n):
  terra_call(para)
...  # continue execution
```

After 1 iteration, program state becomes eq. (1) described above. After 2 iterations, program state becomes

\[
s \land post\text{paras} \land post\text{paras} \land post\text{paras}
\]

This state can be seen by replacing `s` with `s \land post\text{paras}` in eq. (1). After several iterations, the program state will become prohibitively complicated for efficient symbolic execution.

To reduce the verification complexity, CertiQ builds up a library of function calls with a design we call invariant-guided contracts. In the above case, an invariant `invs` becomes a fixed point. In a symbolic execution, a called method with contracts containing only invariant becomes “transparent” where the model checker has a lower verification burden. Invariant-guided contract design tries to implement interfaces that contain needed invariants.

The invariant-guided design is particularly interesting for CertiQ because for every primitive circuit moves in fig. 6, we can find an implementation that has an invariant. For example, the `swap_and_update_gate` method described in §3 has an invariant-guided contract.

To compare with the `basic_swap` function we wrote in the last section, we can look at the current implementation of the `basic_swap` pass in Qiskit Terra:
As we can see, there are two for loops in the outer loop and we cannot perform contract continuation to either loops because the apply_operation_back method and layout swap method does not have invariants in their contract. In general, implementation like this does not scale in symbolic execution.

4.4 Contracts for user defined functions

For user provided functions, CertiQ cannot not specify their contracts. Then the symbolic execution can fail because of the complexity of the code. CertiQ solves this problem in the following order: 1) CertiQ defines several commonly used contracts. With the user writing one line of function annotation, the corresponding pre-defined contract will be applied to the function and be tested if the function complies; 2) If the user does not provide annotation, CertiQ will perform contract continuation for the user function; and 3) If both 1 and 2 fail, the user function will continue with symbolic execution.

Pre-defined 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 ith element and i + 1th element of the returned path must be 1 on the input coupling map.

Contract continuation. If no contract is assigned for a user function, CertiQ will perform contract continuation (invariant continuation). Similar to replacing real implementations with verified contracts, contract continuation can also be viewed as predicate abstraction, but with the possibility of failure. In the following general case, if host_function and guest_func1() and guest_func2() are user-defined functions, and the user provides a contract for the host_function that needs to be verified,

```
# @host_contract
def host_function():
    ... # symbolic execution
guest_func1() ...
    ... # symbolic execution
guest_func2() ...
    ... # other calls
```

If we denote the program state before entering guest_func1() as s, the continued contract for guest_func1() is given by the continuation step at s (denoted as a),

$$as = \{c \in host_inv : cs \land gs \models cgs\}$$

where host_inv is the invariant in the known host contract, gs is the execution of guest_func1() on the program state s. If as is empty, it will be evaluated to ⊥, which means the continuation fails. If the continuation for guest_func1() succeed, the verification engine will try contract continuation on guest_func2(). If contract continuation fails at some point, the verification engine will proceed with symbolic execution. Another contract continuation strategy is that verified contracts can be passed from guest functions to host functions, as described in the example of basic_swap pass in §3. In CertiQ, user is allowed to choose continuation strategies.

4.5 Loops and conditional statements

In CertiQ, we view loops and if statements as user defined functions. Users can provide loop-invariants and if-invariants for their contracts with a single line of annotation. For loops, if no loop invariant is given, CertiQ will try contract continuation. If no contract is assigned at the end of contract continuation, the verification will exit with “fail.” For if statements, if no user provided invariant is given and contract continuation fails, in the static analysis stage, we generate two copies of the code with the if-else code block replaced by the “if” branch and the “else” branch, respectively. The strongest post-condition will then be derived with Z3 tactics to continue the symbolic execution.

4.6 The translation validator

CertiQ also provides a translation validator for swap passes and CNOT optimization passes if the symbolic execution fails. The translation validator can be viewed
as a transformation pass that reverts the changes of the pass it validates and it is also verified by the CertiQ verifier. As an example, we illustrate the validation process of swap passes with an input circuit of 3 qubits in fig. 9. We assume the 3 qubits are coupled linearly, i.e., the coupling map can be represented as \( q_1 - q_2 - q_3 \). For validating swap passes with the input in fig. 9 (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 passes, a similar algorithm is performed.

In the case study described here, we show the process of designing contracts for our verification goals and how it helps identify a bug in the lookahead_swap pass.

There are three verification goals for swap passes:
- The pass must be semantics preserving.
- The output DAGCircuit of the pass must conform to the coupling map of the physical device.
- The pass must terminate.

To prove each verification goal, we design a contract and perform a symbolic execution to verify the contract. The contract for the first goal is demonstrated in §3.2.

For the second verification goal, to ensure that the pass correctly accomplishes its goal of transforming the circuit to match device coupling constraints, we must verify that every 2-qubit gate in the output circuit operates on two neighboring physical qubits. Therefore, the following post-condition is added,

```python
def swap_post(dag, layout, coup):
    n = dag.num_2q_gates()
    i = fresh_int()
    gate = dag.2q_gates[i]
    p1 = layout.v2p(gate.op1())
    p2 = layout.v2p(gate.op2())
    return ForAll([i], Implies(And(0 <= i, i < n),
                               coup.distance(p1, p2) == 1))
```

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

```python
    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. 10). The lookahead_swap pass greedily finds the next best 4 swap gates to minimize the total distance of the unmapped

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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 validate_swap method (which is semantics preserving). After all swap gates are cancelled out by applying the cancel_swap method, we recover the input circuit.

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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. 6, thus gate_remaining.size will not update.

![Diagram showing swap gates]

We next focus on verifying the will not update.

Fig. 10. (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).

5.2 The optimize_1q_gate pass

We next focus on verifying the optimize_1q_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 a primitive merge_1q_gate method. This pass collapses a chain of single-qubit gates into a single, more efficient gate [39], 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.

\[
\begin{align*}
\begin{bmatrix}
1 & 0 \\
0 & e^{i\lambda}
\end{bmatrix}, &
\begin{bmatrix}
1 & -e^{i\lambda} \\
e^{i\phi} & e^{i\lambda+\phi}
\end{bmatrix}, &
\begin{bmatrix}
\cos\theta & -e^{i\lambda}\sin\theta \\
e^{i\phi}\sin\theta & e^{i\lambda+\phi}\cos\theta
\end{bmatrix}
\end{align*}
\]

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

The optimize_1q_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_1q_gate to merge the gates in each group. merge_1q_gate first transforms the single qubit gates from the Bloch sphere representation to the unit quaternion representation [17], then the rotation merges are performed in that representation.

As described in §4.2, 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 [32, 33]. 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. 11. Correct execution (top) and incorrect execution (bottom) of merge_1q_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. 6. First, commutation_analysis transforms the DAGCircuit to a representation called commutation groups [40], where nearby gates that commute with each other are grouped together. Then commutative_cancellation performs cancellation inside groups. In fig. 12, we give a working example.

![Fig. 12. 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.]

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 that the commutation group representation violates contextual refinement property defined in §4.2. This violation comes from the fact that the commutation relation
is in general not transitive. For example, if we denote the commutation relation as $\sim$ and there is 3 quantum gates, $A, B, C$ where $A \sim B, B \sim C$, then $A \sim C$ 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 $\sim$ is indeed transitive. For example, in the gate set \{CNOT, X, Z, H, T, $u_1, u_2, u_3$\}, $\sim$ 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 $\text{gate.c_if==False}$ and $\text{gate.q_if==False}$.

6 EVALUATION

We performed verification of four transpiler phases with seven implementations. The seven implementations are: the collect_q_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. With invariant-guided contract design, all transpiler passes can be verified within seconds. However, most of the original implementations can not 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 CertiQ 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 WORKS

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 [35, 37], programmers can use the embedded verifier based on the Coq proof assistant [7] to perform mechanized proof for their programs. The QST programming environment [25] allows users to reason about their programs written in the quantum while-language with quantum Floyd-Hoare logic [47]. 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], ancillary uncomputation [35, 36] and compiler optimizations [18] utilize interactive theorem provers such as F* [28] 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 [45], 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 CertiQ.

Model checking in quantum computation verification. The early adoption of Model checking in quantum computation focused on verifying quantum communication protocols [10, 16, 43, 48]. Recently, model checking techniques have been applied to more areas, including quantum Markov chain analysis [12–14], checking physical systems, program analysis [21, 24, 49]. However no automated verification tool based on model checking like CertiQ exists for quantum computing until now.

8 CONCLUSION AND FUTURE WORK

We describe CertiQ, a mostly-automated verification framework for the Qiskit compiler (called Terra) that
addresses the key challenges of verifying a real-world quantum compiler. CertiQ gives small-step semantics to quantum circuits for efficient verification of compiler transformations and adapts 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, contract-based design, invariant contracts and contract continuation. With extensive case studies, we demonstrate that CertiQ can detect critical bugs, some of which are unique to quantum software.

To our knowledge, our work with CertiQ is the first effort to apply formal verification and SMT reasoning to 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 [27], which implements quantum operations through microwave control pulses.

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