Quantum computing hardware has progressed rapidly. Simultaneously, there has been a proliferation of programming languages and program optimization tools for quantum computing. Existing quantum compilers use intermediate representations (IRs) where quantum programs are described as circuits. Such IRs fail to leverage existing work on compiler optimizations. In such IRs, it is non-trivial to statically check for physical constraints such as the no-cloning theorem, which states that qubits cannot be copied. We introduce QSSA, a novel quantum IR based on static single assignment (SSA) that enables decades of research in compiler optimizations to be applied to quantum compilation. QSSA models quantum operations as being side-effect-free. The inputs and outputs of the operation are in one-to-one correspondence; qubits cannot be created or destroyed. As a result, our IR supports a static analysis pass that verifies no-cloning at compile-time. The quantum circuit is fully encoded within the def-use chain of the IR, allowing us to leverage existing optimization passes on SSA representations such as redundancy elimination and dead-code elimination. Running our QSSA-based compiler on the QASMBench and IBM Quantum Challenge datasets, we show that our optimizations perform comparably to IBM’s Qiskit quantum compiler infrastructure. QSSA allows us to represent, analyze, and transform quantum programs using the robust theory of SSA representations, bringing quantum compilation into the realm of well-understood theory and practice.

Additional Key Words and Phrases: intermediate representations

1 INTRODUCTION

Quantum computers harness quantum mechanics to perform efficient computation. They are widely believed to be capable of "quantum supremacy" — the ability to perform computations that are not efficiently simulatable using classical computation [Arute et al. 2019]. Due to the rise of Noisy Intermediate-Scale Quantum (NISQ) technology, where we possess quantum computers that are sufficiently powerful to exhibit quantum supremacy [Preskill 2018], there is a growing interest in quantum compiler toolchains that analyze and optimize quantum programs. Quantum computation has quite different semantics from classical computation. Quantum programs operate on quantum bits (qubits), the counterpart to a classical bit. The state of a qubit can be in a superposition between the classical bit states of $|0\rangle$, $|1\rangle$. Other differences from classical computing include the fact that all quantum operations are reversible and that it is impossible to create an independent and identical copy of an arbitrary unknown qubit, as given by the no-cloning theorem [Wootters and Zurek 1982]. These differences make it challenging to analyze and optimize quantum programs.

Designing IRs for quantum programming languages is made more complex due to hybrid quantum-classical programs, where a quantum circuit and a classical computer communicate information to perform computations. To express such computations, we need a single language to express both quantum and classical computation. This is a challenging language design problem that needs an IR design that allows quantum computing and classical computing semantics to interoperate harmoniously in the same IR. Two major classes of quantum programming languages exist. First, quantum compilers for pure quantum programs, which use intermediate representations (IR) where quantum programs are described as circuits. This choice is inspired by the quantum computing literature, where quantum algorithms are commonly analyzed as circuits. The circuit encoding poses two problems. (a) the IR exists as an in-memory DAG with no textual representation. This makes testing, debugging, and interfacing with these compilers challenging. (b) this representation of quantum programs as circuits cannot express hybrid computations. IRs such as Qiskit [Aleksandrowicz et al. 2019], Cirq [Developers 2021], and XACC [McCaskey et al. 2020]
take this choice to represent only pure quantum programs. To cover hybrid quantum-classical programs, IRs such as QIR [Microsoft 2020], Scaffold [JavadiAbhari et al. 2014], QCL [Ömer 1998], and Quil [Smith et al. 2016] attempt to bridge the gap by representing the classical portion with a standard SSA-based imperative IR, and the quantum portion as a special type of “qubit memory”. Instructions that modify qubits are represented as loads and stores into the special qubit memory. The presence of memory operations makes the IR impure due to side-effects. It disables the reuse of standard optimizations across the classical and quantum parts of the IR due to the presence of two different flavors of memory. Furthermore, the use of memory-based qubit semantics forces the use of complicated alias and dataflow analysis to reason about the IR. In summary, pure quantum circuit IRs lack expressivity, while hybrid quantum circuit IRs lack optimisability.

For an optimizable hybrid quantum-classical program IR, we identify four key requirements:
(1) The IR must represent hybrid quantum-classical programs with complete encodings of both classical computation and quantum computation. (2) The IR must naturally express well-known transformations. For example, redundancy elimination is commonly run on the IR for canonicalization as it is an enabling transformation, which makes the IR simpler. For such a transformation to depend on complex static analysis makes the transformation both more expensive (since the static analysis must be computed) and less robust (since the static analysis is an over-approximation). (3) The IR should be as similar as possible to existing compiler IRs to (a) enable the reuse of algorithms and code, and (b) to identify what extensions are necessary for classical compiler IRs to express quantum programs naturally. Finally, to aid compiler debugging, development, and testing. (4) The IR must be easily readable and modifiable for humans. This implies that the IR cannot solely exist as in-memory data structures. The compiler toolchain must be able to dump the in-memory IR into a readable textual format and ingest the textual representation back into the compiler pipeline. This ensures that the textual representation is lossless, which enables modular testing of the compiler. This has been used to great success by LLVM’s FileCheck infrastructure to unit test the entire compiler.

To fulfill the above four criteria, We craft QSSA - an SSA-based IR - to represent and optimize hybrid classical-quantum programs. QSSA expresses the circuit’s data dependencies with the def-use chain of SSA values. Furthermore, since SSA names the outputs of each primitive instruction, it effectively names every edge in the circuit DAG, which aids circuit debuggability. For the hybrid quantum-classical regime, QSSA provides side-effect free, value-semantics based operations for qubit manipulation. This ensures that QSSA’s qubit representation can interoperate with classical SSA analyses. QSSA thus establishes the extensions for SSA necessary to express hybrid programs. To ensure that quantum invariants are preserved, we develop a static analysis that verifies that each qubit is used at most once. QSSA extends the representation used between pure quantum representations - a DAG-based, SSA-like encoding - to the full hybrid quantum representation. We argue that to harness SSA and optimize hybrid quantum-classical programs, we must extend SSA with qubits to preserve value semantics. To our knowledge, this paper is the first to propose this solution. We make the following contributions:

- We define the semantics of quantum-SSA (QSSA), where we identify the extensions necessary for side-effect free SSA to naturally describe hybrid quantum-classical programs.
- We present a novel algorithm to statically verify no-cloning for QSSA, which takes quadratic time on general control flow graphs, and linear time on control flow graphs that preserve high level program structure using regions.
- We translate classical SSA analyses and transformations into the QSSA framework while maintaining quantum invariants.
• We develop a prototype implementation of our proposal in MLIR, a compiler development framework for SSA-based IRs that has built-in support for well-known SSA optimizations, along with an API design that ensures that QSSA has a textual on-disk representation which can be fed back into our compiler pipeline.
• We validate our implementation on the QASMBench [Li and Krishnamoorthy 2020] and IBM Quantum Challenge [QISKit Developer Challenge 2017] datasets, and show that our optimizations perform comparably to IBM’s Qiskit quantum compiler infrastructure.

2 BACKGROUND
This section provides a broad overview of the ideas necessary to appreciate QSSA. It introduces the SSA intermediate representation, the ideas of quantum computing that influence the design of our SSA language, and the MLIR compiler framework for building SSA-based compilers.

2.1 Quantum Computing
In this paper, we deal with discrete quantum systems, which are comprised of qubits. Quantum programs are built by applying gates on these qubits [Nielsen and Chuang 2011, Chapter 4].

2.1.1 Qubits. A Qubit is a two-level quantum system whose state is described by a unit vector in a complex 2D Hilbert space $\mathbb{C}^2$. We consider $\{|0\rangle, |1\rangle\}$ to be the canonical basis of this space. The general state of a qubit is of the form $a|0\rangle + b|1\rangle$ where $a, b \in \mathbb{C}$, $|a|^2 + |b|^2 = 1$. The basis states are analogous to classical bits, but qubits are allowed to take on more states which are superpositions of these basis states. The tensor product of individual qubit states represents the state of a multi-qubit system.

2.1.2 Gates. A gate is a unitary operator acting on the space of states. A gate is analogous to a logical gate in classical computing. On applying a physical gate on a qubit, its state vector gets transformed by the unitary operator. The unitary condition ensures that the resulting state is also a unit vector. Quantum gates can take in any number of qubits as input and return the same number of qubits as output after applying the unitary.

2.1.3 Measurement. To extract the state of a qubit, a measurement is performed. The result of measuring a qubit in the state $a|0\rangle + b|1\rangle$ is a single bit (0 or 1). This operation is probabilistic and produces the bit 0 with probability $|a|^2$, and produces the bit 1 with probability $|b|^2$. The aforementioned condition that $|a|^2 + |b|^2 = 1$ is a condition that ensures that the total probability is always 1. On measurement, the qubit collapses to the measured state, and repeated measurements will give the same result.

2.1.4 The No Cloning theorem. In physics, the no-cloning theorem [Wootters and Zurek 1982] states that it is impossible to create an independent and identical copy of an arbitrary unknown quantum state. This implies that in the compiler IR, we must not allow programs that require multiple copies of the same value. Existing compilers generally enforce this by a run-time check.

2.1.5 Hybrid Classical-Quantum Programs. Quantum circuits consist of a sequence of gates applied on a set of qubits, which are finally measured to extract some result. Frameworks like Cirq are used to express pure quantum circuits. This design is restrictive, as it does not allow any classical feedback to control which quantum gates to apply. Hybrid programs are allow the interleaving of classical computation control flow with quantum operations. This helps describe a larger class of quantum programs. One instance of this is the class of Variational Quantum Algorithms [Cerezo et al. 2020], which uses results of quantum measurements to perform classical computation, which in turn decides which quantum operations to apply next, and so on.
2.2 Quantum Intermediate Representations

We compare our design against two standard quantum IRs: OpenQASM and QIR. These represent extrema in the spectrum of quantum compilation. OpenQASM is a minimal IR designed to represent fixed size, pure quantum circuits. QIR is the IR for Q#, a general-purpose hybrid quantum programming language.

2.2.1 OpenQASM. \(^1\) is a low-level quantum assembly language by IBM [Cross et al. 2017]. It represents universal physical circuits over the CNOT plus SU(2) basis with straight-line code. It has support for measurement, reset, and gate subroutines. It uses memory semantics to represent qubit manipulation. OpenQASM has been designed for the representation and optimization of pure quantum circuits. Thus, OpenQASM acts as an anchor throughout the paper to discuss pure quantum circuits and qubit-memory based semantics.

We briefly describe its instructions that are used in the paper. Fixed-size qubit registers are allocated using the `qreg` instruction. For example, `qreg q[4];` declares a register of 4 qubits. Similarly, `creg` allocates a fixed-size classical register of bits. A gate application is like a function call - the name of the gate followed by qubit arguments. For example, to apply the CNOT gate, we write `cx q[0], q[1];`. The `measure` instruction measures a qubit/qubit register and stores it in a classical register. `measure q[0] -> c[0];` stores the measurement result of `q[0]` in `c[0]`.

2.2.2 QIR. is an LLVM-based IR for hybrid quantum programs [Microsoft 2020]. QIR is the compiler intermediate target for Q#, a hybrid quantum programming language by Microsoft. QIR extends LLVM with opaque intrinsics to represent qubits and qubit arrays as opaque pointer types. QIR’s encoding of LLVM does not interoperate with the rest of the LLVM language, as we will demonstrate in Section 4.2. Thus, QIR acts as an anchor throughout the paper to discuss hybrid classical-quantum programs, as well as issues with mixing classical and qubit memory semantics.

2.3 Static Single Assignment

An intermediate representation (IR) is in static single assignment form (SSA) [Rastello 2010] if each variable is assigned exactly once and no variable remains undefined. SSA has gained popularity in imperative compilers such as GCC [Stallman 2002], LLVM [Lattner and Adve 2004], and many others, as data-flow information is explicitly expressed through dependencies from the definition of a value to its uses (def-use chains). SSA-based IRs typically use basic blocks that hold lists of sequentially executed operations, each taking a list of argument values and returning a tuple of return values. Terminator operations at the end of each basic block, which either branch to another basic block or return from a function, combine these basic blocks into a control flow graph (CFG). While IRs typically use a flat CFG, MLIR [Lattner et al. 2021] recently introduced nested control flow as a first-class concept to support abstractions that require control over scope. Operations can now receive `regions`, which are nested single-entry sub-CFGs, as additional arguments. Regions make it easy to express concepts such as loop bodies or branches of an if-statement.

2.4 MLIR

MLIR is a new compiler infrastructure under the LLVM umbrella [Lattner et al. 2021]. It aims at simplifying development domain-specific compilers. For this, MLIR provides a non-opinionated, SSA-based intermediate representation (IR). Having a customizable IR allows compiler developers to model domain-specific concerns by introducing custom types, operations, and attributes. Here, we briefly describe the relevant aspects of MLIR that are used in our compiler.

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\(^1\)In this paper, OpenQASM refers to version 2.0. At the time of writing, version 3.0 is under development, which does not change the core characteristics of the IR.
2.4.1 Modules. Each program in MLIR is called a Module. A Module consists of several global functions. Function names such as @foo are global and allow for linking function calls across modules. A function consists of a sequence of SSA operations. Each SSA value is local to the scope of the function and has a name of the form %bar.

2.4.2 Operations. SSA values are produced by Operations, such as addi, which stands for the integer addition operation. Each operation takes zero or more SSA operands that are defined before it and returns zero or more SSA values. Operations can also have compile time constants attached to them, such as {phase = 90.0 : f64}. These are called attributes.

2.4.3 Dialects. A Dialect in MLIR is a collection of operations and types of a certain kind. In this paper, we use two existing dialects, std and scf. The std dialect contains all basic operations such as constant declarations, arithmetic operations and memory manipulation. The Structured Control Flow Dialect scf contains if-else and for loop constructs.

3 THE QSSA REPRESENTATION
This section describes the QSSA Intermediate Representation, prototyped as an MLIR dialect. The aims of the encoding are twofold: (1) Encode all qubit operations using value semantics, thereby making the program side effect free, and (2) Exploit the SSA def-use chain to encode the quantum circuit within the IR implicitly.

Consider the program in Figure 1. We first allocate a qubit array at 1 using the qssa.allocate instruction to allocate an array of 3 qubits. We wish to isolate the first two qubits from the array of three qubits to apply a Controlled-X operation on them. To do this, we break apart the 3 element array into a (2 element, 1 element) pair using the qssa.split instruction at 2. We dispatch the qubit pair to a Controlled-X operation at 3 with call. 4 decomposes the two-qubit array further into a pair of single qubits, 5 invokes an inbuilt CNOT instruction, and 6 puts back the pair of two single qubits into a two-qubit array with qssa.concat. We return control flow back to the main program at 7. Next, we put back the original three qubit array with another call to qssa.concat at 8. Finally, we measure the state of all three qubits with qssa.measure to convert...
define void @testground__cx__body(%Array* %qs) {
  entry:
  %0 = call i8* @qntmGep(%Array* %qs, i64 0)
  %1 = bitcast i8* %0 to %Qubit**
  %2 = load %Qubit*, %Qubit** %1, align 8
  %3 = call i8* @qntmGep(%Array* %qs, i64 1)
  %4 = bitcast i8* %3 to %Qubit**
  %5 = load %Qubit*, %Qubit** %4, align 8
  call void @qntmIntrinsicCNOT(%Qubit* %2, %Qubit* %5)
  ret void
}

define void @testground__main__body() {
  %qs = call %Array* @qntmAllocateQubitArray(i64 3)
  %0 = load %Range, %Range* @EmptyRange, align 4
  %1 = insertvalue %Range %0, i64 0, 0
  %2 = insertvalue %Range %1, i64 1, 1
  %3 = insertvalue %Range %2, i64 2, 2
  %4 = call %Array* @qntmArraySlice1d(%Array* %qs, %Range %3, i1 false)
  call void @testground__cx__body(%Array* %4)
  %bases = call %Array* @qntmArrayCreate1D(i32 1, i64 3)
  ... %res = call %Result* @qntmMeasure(%Array* %bases, %Array* %qs)
  ret void
}

Fig. 2. Example program contrasting QIR with QSSA. All quantum operations are encoded using memory-based semantics.

qubits into classical measurements at 9. There is an explicit one-to-one correspondence between the program and the quantum circuit it describes, as seen in Figure 1. The circuit has two physical operations, CNOT and measure, and the rest describe the mapping between the physical qubits and the QSSA qubits arrays.

We contrast this to the QIR program in Figure 2. First, the array of three qubits is allocated at 1 with a call to an intrinsic qntmAllocateQubitArray 2 which returns a *pointer* to an array. Next, the @EmptyRange global is accessed at 2 with a load instruction, which manipulates global memory, modeled as a *pointer load*. Next, the array is filled with empty qubits, after which a call is made to invoke the cx function at 3. Lines 5, 6 first construct an offsetted *pointer* with qntmGep and then load the value pointed to with a load instruction at 6. Note that the value loaded, %2, ostensibly is a qubit and yet is modeled as a *pointer to a qubit*. Similarly, line 7 also loads from a pointer. Finally, the intrinsic qntmIntrinsicCNOT is invoked at 8 to compute a CNOT operation. No value is returned back to main, since the quantum semantics are modeled based on side-effects. Finally, at 9, we measure the qubits with a call to the intrinsic qntmMeasure.

We see that throughout, QIR uses pointer based, side-effecting semantics rather than value-based non side-effecting(pure) semantics. Since QIR is implemented as an extension of LLVM, it implements quantum operations by hiding the semantics of the quantum intermediate representation behind *opaque pointers*. This process, by construction, inhibits LLVM’s ability to reason about the QIR encoding, as the value semantics of modifying qubits is complexified into the pointer semantics of manipulating an opaque pointer with a function call. Hence, QIR is hard to analyze and optimize.

In contrast, we see that QSSA provides value semantics and pure computation, which aids analysis and optimization, as we will see in Section 4. Now that we have seen a representative

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2Names are changed for brevity. Code is left unaltered.
example of QSSA, we shall survey the type system, instructions, and single-use constraints of the IR.

### 3.1 Type system
QSSA has a qubit array type called qubit<>. The array can be either statically sized, represented as qubit<10>, or dynamic sized, represented as qubit<?>. We support dynamically sized arrays to express functions that are generic over the size of the array, as described later in Figure 3.

### 3.2 Classical Operations
We use MLIR’s std for classical arithmetic and logical operations. We use MLIR’s scf dialect, which provides scf.if and scf.for, which encodes high-level control flow directly within the intermediate representation with the use of regions.

### 3.3 Quantum Operations
QSSA has operations for (1) allocating qubits, (2) applying gates to qubits, (3) measuring qubits to extract classical bits, (4) manipulating qubit arrays while preserving the single-use semantics.

#### 3.3.1 Allocation
qssa.alloc allocates an array of qubits of fixed or variable length.

```plaintext
%q = qssa.alloc : qubit<10>
```

#### 3.3.2 Gate Application
We provide a complete basis set of quantum gates\(^3\), given by:

- qssa.CNOT: The controlled NOT gate.
- qssa.X, qssa.Y, qssa.Z: The X, Y, Z Pauli gates.
- qssa.H: The Hadamard gate.
- qssa.Rx, qssa.Ry, qssa.Rz: Rotation gates that rotate about the X, Y or Z axis by a given angle.
- qssa.S, qssa.Sdg, qssa.T, qssa.Tdg: The Phase Gate, T Gate, and their adjoints.
- qssa.gate, qssa.U: As there are many possible choices of universal gate sets for quantum programs [Deutsch et al. 1995], we provide a generic instruction to define arbitrary gates. These can be used to define gates by specifying their matrix form. The \(U\) gate is a convenience to describe an arbitrary single-qubit unitary by specifying its ZYZ Euler angles.

#### 3.3.3 Measurement
The qssa.measure operation takes a qubit array, measures the qubits in the standard (Pauli-Z) basis and returns the results as a 1D tensor of bits (i1), along with the qubits.

#### 3.3.4 Array Manipulation
All QSSA operations receive qubit arrays as input. To support slicing and indexing arrays without losing our single-use constraint, we provide four primitives: qssa.split, qssa.concat, qssa.dim and qssa.cast

- qssa.split takes a qubit array and returns the split into two parts. The sizes of the two parts are indicated in the return type.
- qssa.concat takes two qubit arrays and concatenates them into a single qubit array.
- qssa.dim takes a qubit array and returns its size and the array itself.
- qssa.cast takes a qubit array and casts it to a different type. This can be used to cast a static array to a dynamic one, or vice versa.

Consider the program in Figure 3. The function @applyXOnLast \(^4\) takes a dynamic sized qubit array and applies X on the last qubit in the array. We allocate a three qubit array \(^2\), and cast it to a dynamic qubit array type \(^3\). The converted qubit array is now passed to the function at \(^4\). In the function @applyXOnLast, we first get the dimension of the argument \(^5\). We then subtract one

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\(^3\)For a full reference of the gates and their matrices, refer to [Nielsen and Chuang 2011, Nomenclature and notation]
func @applyXOnLast(%qs : qubit<?>) -> qubit<?> {
  %qs1, %n = qssa.dim %qs : qubit<?>
  %1 = constant 1 : index
  %n_1 = subi %n, %1 : index
  %qs2, %ql = qssa.split(%n, %n_1) : qubit<?> -> (qubit<?>, qubit<1>)
  %ql1 = qssa.X %ql : qubit<1>
  %qs3 = qssa.concat %qs2, %ql1 : (qubit<?>, qubit<1>) -> qubit<?>
  return %qs3 : qubit<?>
}

func @main() {
  %qs = qssa.alloc : qubit<3>
  %qs1 = qssa.cast %qs : qubit<3> -> qubit<?>
  %qs2 = call @applyXOnLast(%qs1) : (qubit<?>) -> qubit<?>
  return
}

Fig. 3. Example QSSA program showing dynamic sized qubit arrays and the array manipulation operations

from it at 6, to compute the size of the left side array. We then call split at 7, passing n and n – 1 to it, which correspond to the sizes of each of the dynamic arrays in the type signature. We then apply X on the last qubit, and concatenate them back at 8.

3.4 Semantics: Side-effect free operations

All QSSA operations (except alloc) have no side-effects. They take input qubits, operate on them and return the resulting qubits - which effectively correspond to the same physical qubits in the underlying system. We explain how this enables us to reuse SSA optimization in Section 4.3

3.5 Single Use Analysis

Each SSA value representing a qubit must be used only once to enforce the no-cloning constraint. We describe an analysis for an SSA-based IR with CFGs that enforces this constraint. We then adapt this analysis to MLIR, which offers nested CFGs using regions.

3.5.1 Algorithm for flat CFG. In this scenario, we consider a CFG with no cycles. For each qubit SSA value %q, consider all uses. (1) If a use is within the same basic block, then the qubit is dead, and we check that there is no other use in any other basic block. (2) If there are uses in other basic blocks, then for every pair of uses 𝑢_𝑖 and 𝑢_𝑗, we check that there is no path from 𝑢_𝑖 to 𝑢_𝑗 and vice versa. This can be done in linear time using dynamic programming on the CFG DAG. We process the blocks in reverse topological order. If the block has a use of the qubit, we mark the block as used. If any child block has been marked, then we mark the current block as well. If the block gets marked twice, then there is a repeated use.

3.5.2 Adaptation to Regions. Regions can be used to represent higher-level control flow constructs. Representing control flow such as if conditions and while  loops directly in the IR allows us to infer facts about control flow without building and querying the dominator tree, as we would have to for an arbitrary CFG. We exploit this to optimize our single-use analysis by assuming a regular program structure that consists of only a single basic block, with all control flow represented by nested regions using scf.if (if-then-else), and scf.for (for loops). This allows us to deduce a linear time algorithm to verify single-use.

Constraints. We must verify the following constraints: (1) A qubit can be used at most once in the same region. (2) If the qubit has two uses in different regions, then neither region must be an
QSSA

1. SINGLE BASIC BLOCK
   
   ```
   %0 = qssa.alloc
   ...
   %1 = qssa.X %0
   ...
   ```

   Single use of %0.
   Correct

2. SCF.IF
   
   ```
   %0 = qssa.alloc : qubit<1>
   %1 = scf.if %b -> qubit<1> {
      ...
   } else {
      ... Recursively analyze:
      At most one %0 use
   }
   ```

   Multiple uses of %0.
   Incorrect

3. SCF.FOR
   
   ```
   %0 = qssa.alloc : qubit<1>
   %1 = scf.for ... {
      ...
   }
   ... Recursively analyze:
   No %0 use
   ```

   No use of %0.
   Correct

4. Recursively analyze:
   
   ```
   %0 = qssa.alloc
   ...
   %1 = qssa.X %0
   ...
   %2 = qssa.X %0
   ```

   Use of %0.
   Incorrect

Fig. 4. Linear time algorithm to determine qubit single-use in a program with straight line code, and control flow represented using scf.if, scf.for

Algorithm. We consider the topmost region (could be a function body) which is isolated from above. We perform a depth first search from this root region on the region tree induced by the control flow operation. We maintain two sets of qubits: ones that are defined but not used \( D \), and ones that are used - \( U \). At each region \( R \), we perform the following:

1. Maintain a set \( B \) for rolling back updates.
2. Iterate through the operations linearly. For each operation, we verify that all its qubit arguments \( q \) lie in \( D \). If so, we move \( q \) from \( D \) to \( U \), and add \( q \) to \( B \).
3. For all the scf.if operations, recursively verify the constraints, by passing the sets \( D' = D, U' = U \).
4. For all the scf.for operations, recursively verify the constraints, by passing the sets \( D' = \) iter_args, \( U' = \{ \} \).
5. Rollback all the qubits in \( B \), by moving them from \( U \) to \( D \).

4 QSSA OPTIMIZATIONS

QSSA allows us to easily adapt many classical SSA analyses and optimizations to the quantum regime. Here, we outline both our single-use analysis, as well as adaptations of classical SSA transforms such as common sub-expression elimination.
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4.1 Peephole Optimizations

QSSA provides classical peephole optimizations on the quantum circuit, where we look for sub-circuit patterns, and then replace matches with a more optimized version of the sub-circuit being matched. The purity of our IR enables us to pattern-match and rewrite directly on the SSA DAG, since we can ignore the ordering of instructions as there are no side effects. An example transformation in Figure 5 we perform, the Pauli X gate is a self-inverse. Thus, applying the Pauli gate twice can be optimized away into a no-op. This can be concisely stated using the MLIR pattern matching framework, as the data dependencies are encoded.

In total, we implement the following matrix identities:

1. CNOT-CNOT optimization.
2. \( U \) gate merging.
3. Pauli relations: \( X^2 = Y^2 = Z^2 = -iXYZ = I \).
4. Hadamard self-adjoint: \( H^2 = I \).
5. Drop phase before measurement.

Our implementation of these peephole optimizations is declarative. This is in contrast to Qiskit, where the optimization passes are written in imperative Python code that manipulates internal data structures. We use MLIR’s TableGen infrastructure to declare DAG-to-DAG rewrites, which are then automatically applied during canonicalization. Figure 6 showcases a few examples of the above mentioned rewrite patterns.
4.2 Redundancy Elimination

QIR and QSSA model qubits with side-effecting memory operations and how this inhibits optimizing code where qubits may alias. In contrast, QSSA trivially exploits SSA’s redundancy elimination to optimize examples that QIR is unable to.

In Figure 7, we consider redundancy elimination for QIR. We should be able to hoist the operation \( H(q[0]) \) in the then and the else branch, at locations 1 and 2 since it occurs in both branches of the Q# source code. The generated QIR occludes the transformation by using array indexing semantics with \( \text{qntmGep} \) at 3, 4, 5 in the then branch, and similarly in the else branch. Hoisting the \( H(q[0]) \) instruction encoded by \( \text{call void @qntmH(%Qubit* %q2)} \) requires alias analysis to ensure that the qubit \( %q2 \) does not alias with \( %q1, %q3 \). QIR is unable to perform this alias analysis and is thus unable to optimize this program 4. In contrast, the QSSA pipeline shown in Figure 8 explicitly encodes qubit dependencies in the def-use chain. It is clear that the \( \text{qssa.H} \) instructions have the dependency chain 2 \((a2 \mapsto a1) 1\). The hoisting analysis ignores the interleaved \( %b2 = \%\text{qssa.X}(%b1) \) instruction. This allows QSSA to hoist the instruction out of the \text{scf.if}, as shown at 4. This optimization is performed entirely by the inbuilt global value numbering pass, aided by our SSA encoding of quantum semantics.

4.3 Reusing SSA optimizations

All quantum operations except \text{alloc} have no side-effects. That is, the results of such an operation is completely determined by its inputs, and it does not depend on any external state, nor does it change it. The Allocate operation \text{alloc} has a minor side-effect just like a memory allocate instruction (eg. \text{malloc}). It acquires a resource but does not modify it. We only allow optimization passes that do not create copies of SSA values, since these preserve no cloning. Thus, we reuse:

---

4We generate QIR from Q#, and then optimize using opt -O2, on Q# version Microsoft.Quantum.Sdk/0.15.2103133969, LLVM version 11.1.0
operation hoistH(q : Qubit[], b : Bool) : Unit {
  if (b) { X(q[1]); H(q[0]);   X(q[1]); }
  else   { Z(q[1]); H(q[0]);   Z(q[1]); }
}

define void @hostH(%Array* %q, i1 %b)
entry:
  br i1 %b, label %then, label %else
then:
  %2 = call i8* @qntmGep(%Array* %q, i64 1)
  %3 = bitcast i8* %2 to %Qubit**
  %q1 = load %Qubit*, %Qubit** %3
  call void @qntmX(%Qubit* %q1)
  %4 = call i8* @qntmGep(%Array* %q, i64 0)
  %5 = bitcast i8* %4 to %Qubit**
  %q2 = load %Qubit*, %Qubit** %5
  call void @qntmH(%Qubit* %q2)
  %6 = call i8* @qntmGep(%Array* %q, i64 1)
  %7 = bitcast i8* %6 to %Qubit**
  %q3 = load %Qubit*, %Qubit** %7
  call void @qntmX(%Qubit* %q3)
  br label %continue

else:
  %8 = call i8* @qntmGep(%Array* %q, i64 1)
  %9 = bitcast i8* %8 to %Qubit**
  %q4 = load %Qubit*, %Qubit** %9
  call void @qntmZ(%Qubit* %q4)
  %10 = call i8* @qntmGep(%Array* %q, i64 0)
  %11 = bitcast i8* %10 to %Qubit**
  %q5 = load %Qubit*, %Qubit** %11
  call void @qntmH(%Qubit* %q5)
  %12 = call i8* @qntmGep(%Array* %q, i64 1)
  %13 = bitcast i8* %12 to %Qubit**
  %q6 = load %Qubit*, %Qubit** %13
  call void @qntmZ(%Qubit* %q6)
  br label %continue

May-Alias: cannot hoist %4, %10 without further analysis

Fig. 7. A QIR program where the compiler is unable to hoist the call H(q[0]) due to potential aliasing of array indexes in the IR. The LLVM getelementptr instruction is adapted to qntmGep, an opaque intrinsic whose semantics LLVM does not know. Similarly, the types Array and Qubit are also opaque LLVM types, whose contents and semantics are unknown to LLVM by design. QIR does not interoperate with the LLVM infrastructure, making alias and side-effect analysis impossible, thereby preventing any SSA-based optimization from being performed.

- Inlining
- Loop Unrolling
- Dead code elimination
- Common sub-expression elimination

5 RAISING AND LOWERING

In this section, we describe how our QSSA interacts with non-SSA languages. We describe how we raise OpenQASM, a low-level non-SSA-based quantum IR into QSSA for analysis and optimization. We then describe how to lower QSSA code to OpenQASM.

5.1 Raising OpenQASM to QSSA

To raise from OpenQASM to the QSSA IR, we perform an analogue of mem2reg to convert memory references into SSA def-use chains. To make the conversion simpler, we provide a qasm dialect in MLIR, which is a 1-1 mapping of the OpenQASM operations. The OpenQASM code is first converted to MLIR, using the quantum operations of the qasm dialect, and the classical operations of the std and scf dialects.

5.1.1 Latest Qubit Map. We maintain a map data-structure M that maps each OpenQASM qubit to its latest SSA result that refers to this qubit. When an operation is applied on this qubit, we update the map with the new result. This enables us to do the mem2reg transformation.
Fig. 8. A QSSA program that exhibits redundancy elimination. QSSA expresses data dependencies in the use-def chain, and has no side effects, thus allowing global value numbering to hoist the instruction out of the branch.

Fig. 9. Sample program showing conversion from OpenQASM to QSSA. We first embed OpenQASM within MLIR, after which we perform a mem2reg-like pass to raise qubit memory operations into SSA. New values that are inserted during mem2reg are highlighted in green.

5.1.2 Quantum Registers. As OpenQASM only allows statically sized arrays, we simplify the conversion by allocating single qubits - instead of allocating a qubit array and then splitting. This removes unnecessary split and concat operations. In Figure 9, we convert the two qubit register q[2] to two qasm.alloc operations. We also initialize M[%q0] := %q0 and M[%q1] := %q1.

5.1.3 Gates. To convert a qasm gate, we first extract the latest SSA qubits for each of the gate’s operands. We emit an qssa gate operation with those SSA qubits as inputs, and update the map with the results. In Figure 9 to convert the qasm.H %q0 operation, we emit %q0_1 := qssa.H %q0 and update the qubit map M[%q0] := %q0_1. (Note that %q0_1 corresponds to physical qubit q[0] in the OpenQASM code.)
5.1.4 Measure. In the MLIR qasm dialect, we decouple the measurement and store operations. qasm.measure takes a qubit and returns a bit, and then it is stored in the memref by an explicit store operation. We convert this to QSSA similar to converting gates - measure operation is syntactically like a gate, which returns an extra bit (along with the input qubits).

5.2 Lowering QSSA to OpenQASM

To lower, we first convert all operations in the qssa dialect to the qasm dialect. Then we directly translate all qasm operations to OpenQASM operations.

```
qreg q0[1];
qreg q1[1];
creg c[2];
h q0[0];
cx q0[0], q1[0];
z q1[0];
measure q0 -> c[0];
measure q1 -> c[1];
```

Fig. 10. Sample program showcasing conversion from QSSA to OpenQASM. We first lower from QSSA to MLIR-QASM by eliminating qubit registers. We then translate MLIR-QASM into QASM. The two physical qubits in the program are color coded as light green and dark red respectively.

5.2.1 Allocation. qssa.alloc operations are directly converted to qasm.alloc. Classical registers are identified by memref of type i1. We declare cregs for each of those memref.alloc operations.

5.2.2 Gates. A gate operation is converted by removing its return values. Instead, we replace its current return values with its operands in the rest of the IR. In Figure 10, we convert the `%q0_1 = qssa.H %q0` instruction to `qasm.H %q0`. And then we replace the result `%q0_1` with the operand `%q0` at the qssa.CX.

5.2.3 Measurement. We convert measure operations similarly. As measurements only return the measurement outcome, to convert to OpenQASM, we find which qubit’s measurement result is stored in the memref, and emit the corresponding operation.

6 EVALUATION

In this section, we evaluate our prototype against Qiskit, IBM’s quantum computing infrastructure by measuring optimizations in terms of gate count and circuit depth reduction on two datasets: QASMBench [Li and Krishnamoorthy 2020] and IBM Quantum Challenge Dataset [QISKit Developer Challenge 2017].

QSSA has a set of generic optimizations derived from SSA, along with peephole optimizations described in Section 4.1. We compare our prototype implementation against Qiskit’s standard optimizer [Qiskit 2021], and compute percentage reduction in gate counts from the baseline. We
run Qiskit at three levels of optimization - O1, O2, O3.\(^5\) We compare them using two metrics: (1) percentage number of gates reduced and (2) compilation/optimization time.

### 6.1 QASMBench

QASMBench is a low-level QASM benchmark suite for NISQ evaluation and simulation. It contains 60 programs split into three categories: small (30), medium (16), large (14).\(^6\) It collects common quantum algorithms and routines from a variety of domains including chemistry, simulation, linear algebra, searching, optimization, quantum arithmetic, machine learning, fault tolerance, and cryptography.

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\(^5\)Qiskit supports another level for optimization - level 0 - but we omit it as it does no optimization.

\(^6\)We remove two extremely long programs which contain >2M lines each.
Figure 11 plots a cumulative histogram of the logarithm of gate count and circuit depth of the dataset. The average gate count is 780 and average circuit depth is 252. The dataset is quite extensive, as it covers the number of qubits ranging from 2 to 60K, and the circuit depth from 4 to 12M.

We run the optimizers and plot the final gate counts in Figure 12. We observe that we optimize better than Qiskit level 1 in 30 cases (50%), and achieve parity in 56 out of 60 cases (93%). Compared to Qiskit level 2, we optimize better in 21 cases (35%) and achieve parity in 43 cases (72%). Compared to Qiskit level 3, we optimize better in 18 cases (30%) and achieve parity in 35 cases (58%).

Figure 13 shows the corresponding speedups in compilation times when compared to Qiskit O3. QSSA performs comparably with O1, with a maximum of 2x slowdown in most cases. It also has a 2-3x speedup over O2 in most cases. In some extreme cases - medium VQE and large Ising Model, QSSA performs extremely well with huge speedups over Qiskit - 65x and 44x respectively against O3 and 21x each against O2.

6.2 IBM Quantum Challenge Dataset

The IBM Quantum Challenge Dataset consists of 141 quantum programs, designed to be complex programs to stress test quantum optimization and quantum qubit routing algorithms.7

We begin by characterizing the dataset, and we find that the average gate count is 2198, and average gate depth is 1185. This indicates that our programs are quite large. Figure 14 plots a histogram of the logarithm of the gate count and gate depth of the dataset. We see that there are quite a few large programs, with gate depths of $10^4$.

Figure 15 shows the optimization ratios of the dataset. 5 out of 149 programs get heavily optimized out by Qiskit O3, with optimization ratios between 50%-95%. The three Ising Model programs get optimized to about 50%, and the two QFT programs get optimized to 89% and 95% respectively. We cap the Y-axis at 35% in the plot to improve visualization. QSSA achieves parity in all test cases when compared with Qiskit O1. It achieve parity with 125 out of 149 cases (83%) compared against both O2 and O3. We are performance comparable with the Qiskit optimizer, without any sophisticated rewrites in the QSSA system. We rely purely on peephole rewrites along with standard SSA optimizations. The Qiskit compilation suite is mature, and QSSA being performance comparable showcases the strengths of an SSA-based encoding.

7We remove extremely large programs from the dataset, which being synthetically generated have a size of over $10^6$ lines.
Fig. 14. Cumulative histogram of gate depth and gate counts for the IBM Challenge dataset. We see that the set of programs is quite exhaustive, containing both small and large programs.

Fig. 15. Optimization ratios of the IBM Challenge dataset, which are calculated as the proportion of instructions removed: $1 - \frac{i_f}{i_0}$ where $i_0$ is the initial gate count, and $i_f$ is the final gate count. The x axis is in the ascending order of program length. The y axis is capped at 35% for better visualization. 5 test files exceed the 35% ratio.

We plot compilation/optimization time speedups in Figure 16. We split the dataset into two parts: one with small programs ($\leq 6000$ gates, 133 files) and one with large programs ($> 6000$ gates, 16 files). We consider the speedup over O2 and plot qssa against O1 as it is the extreme (fastest) case. There is an anomaly in really small tests, where O2 is faster than O1. We conjecture that this is due to O2’s awareness of certain patterns which occur in small test cases that enable it to rapidly optimise the test case. (1) In the small set, qssa is faster than O1 in all programs, and faster than O2 in 96% of them. It also has 2x speedup over O1 in 44% of the programs and over O2 in 88% of the programs. (2) In the large set, qssa is 2x faster than all programs over both Qiskit levels. Moreover, it is 5x faster than O2 for all programs. It is also 3x faster than O1 in 62.5% of the programs. In summary, we find that our QSSA optimizer prototyped in MLIR is competitive both in terms of optimizing gate count and compilation time.
Fig. 16. Compilation/optimization speedup of the IBM Challenge dataset. The x axis is in the ascending order of program length. QSSA is faster than O1 and O2 in almost all cases.

7 RELATED WORK

The discovery of efficient quantum algorithms by Shor and Grover led to a proliferation of quantum programming languages [Miszczak 2011]. Cross et al. [2017] introduced OpenQASM - a quantum assembly language to describe quantum circuits using straight-line code. Smith et al. [2016] introduced Quil - a practical quantum instruction set architecture - which can be used to describe quantum programs with classical control flow. JavadiAbhari et al. [2014] introduced Scaffold, an imperative programming model inspired by classical high-level programming languages such as C and C++. It comes with a toolchain based on the LLVM compiler infrastructure, where quantum gates have been modeled using custom intrinsics and qubit using a custom datatype. Microsoft [2020] introduced QIR, an LLVM based IR for the Q# programming language. It uses LLVM intrinsics to model quantum operations and memory semantics to model qubit arrays. McCaskey and Nguyen [2021] have prototyped common quantum assembly languages in MLIR. It models qubits using memory semantics - similar to QIR. The above IRs use memory semantics for qubits and side-effecting quantum operations, which make reusing existing classical compiler optimizations challenging. McCaskey et al. [2020] introduced XACC - a System-Level Software Infrastructure for Heterogeneous Quantum-Classical Computing. Cirq is a framework by Google Quantum AI to represent and transform quantum circuits [Developers 2021]. Aleksandrowicz et al. [2019] introduced Qiskit, which stores circuits using an in-memory DAG representation. The use of in-memory representations makes scaling and reuse of existing compiler infrastructure challenging. Altenkirch and Grattage [2005] introduced QML - a functional language for finite quantum programs QML with an accompanying compiler based on Haskell. It uses first order strict linear logic to describe quantum computation. Green et al. [2013] introduced Quipper - a scalable, functional, higher-order quantum programming language. It is geared towards a model of computation that uses a classical computer to control a quantum device. Silq is a high-level quantum language with safe uncomputation and intuitive semantics Bichsel et al. [2020]. It has a strong static type system to enforce physical constraints. We believe that QSSA is the ideal optimizing IR for such languages, as SSA is effectively a functional language [Appel 1998], and it brings a host of optimization opportunities to them. Schuiki et al. [2020] introduce an SSA-based multi-level IR for hardware description languages. It is used to design classical circuits, which have some similarities to quantum circuit design and analysis. We acknowledge concurrent work by Ittah et al. [2021] which designs a similar IR for optimizing quantum programs.
8 CONCLUSION

Prior work on developing IRs for hybrid quantum-classical programs has focused on adapting classical compiler technology to the quantum regime. However, the translations have ignored the necessary adaptations necessary to exploit SSA’s representational power. We present QSSA, SSA-based IR for representing hybrid quantum-classical programs. We model all quantum operations using side-effect SSA value semantics. This allows us to reuse well known SSA analyses and optimizations, thereby allowing us to leverage the extensive research into SSA optimization. We demonstrate the effectiveness of our approach by evaluating our compiler infrastructure against the QASMBench and IBM Quantum Challenge Datasets, where we achieve performance parity with Qiskit’s optimization pipeline. QSSA enables quantum compilation technology to use decades of SSA research, such as tools like Alive [Lopes et al. 2015] to verify quantum optimizations, and stochastic superoptimizers like STOKE [Schkufza et al. 2013] to discover novel quantum optimizations. In conclusion, QSSA allows us to represent, analyze, and transform quantum programs using the robust theory of SSA representations, bringing quantum compilation into the realm of well-understood theory and practice.

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