We present a multilevel quantum–classical intermediate representation (IR) that enables an optimizing, retargetable compiler for available quantum languages. Our work builds upon the multilevel intermediate representation (MLIR) framework and leverages its unique progressive lowering capabilities to map quantum languages to the low-level virtual machine (LLVM) machine-level IR. We provide both quantum and classical optimizations via the MLIR pattern rewriting subsystem and standard LLVM optimization passes, and demonstrate the programmability, compilation, and execution of our approach via standard benchmarks and test cases. In comparison to other standalone language and compiler efforts available today, our work results in compile times that are $1,000 \times$ faster than standard Pythnic approaches, and $5–10 \times$ faster than comparative standalone quantum language compilers. Our compiler provides quantum resource optimizations via standard programming patterns that result in a $10 \times$ reduction in entangling operations, a common source of program noise. We see this work as a vehicle for rapid quantum compiler prototyping.

Quantum acceleration of existing scientific computing workflows has the potential to enhance computational scalability for modeling and simulation tasks in fields, such as nuclear physics, chemistry, and machine learning. As hardware architectures continue to scale and improve—enabling more qubits at lower error rates—one can expect quantum–classical machine models to move toward tighter integration of central processing unit (CPU) and quantum processing unit (QPU) resources. These architectures stand to benefit from robust language and compilation approaches that enable high-level classical language integration, quantum and classical compiler optimization techniques, and compiler-automated circuit synthesis strategies. There is a critical need to move the quantum programming community from manual circuit construction via vendor-provided data structures and frameworks embedded in application-level classical languages (Python, etc.) toward performant language approaches that enable tight integration with existing classical runtimes, libraries, and languages. Recently, a number of such language approaches have begun to bridge this gap in the research community, with standalone languages, such as Q#, OpenQASM 3.0, Silq, Scaffold, and classical language extensions like QCOR.

In parallel to quantum programming research and development, there has been a wealth of work done to improve classical compilation frameworks and techniques. One result of note is the introduction...
of multilevel intermediate representations (MLIR) enabling compiler representations at a variety of abstraction levels—including those close to the source language itself—in tandem with associated progressive lowering workflows that take high-level representations to low-level executable object code via a hierarchy of intermediate representation (IR) abstraction. This enables robust compiler development for domain specific languages that retain automated language-level optimizations, transformations, and lowering to machine-level IRs, such as the low-level virtual machine (LLVM). Treating quantum program expressions as standalone domain specific languages represents an opportunity to leverage these state-of-the-art classical MLIR. Specifically, the MLIR framework\(^\text{13}\) is an example of a popular MLIR in use today for classically accelerated heterogeneous workflows,\(^\text{4,7}\) and is well-positioned to provide a unique resource for the rapid prototyping of quantum language compilers via its extensible language-level IR and progressive IR-lowering capabilities.

We recently demonstrated the utility of MLIR for simple quantum assembly languages with no true control flow structures—a low level MLIR dialect for quantum computing. In this work, we leverage and extend that simple quantum MLIR extension for a more complex quantum language—OpenQASM version 3.0\(^\text{3}\) (henceforth referred to as OpenQASM, unless stated otherwise), which provides robust control flow structures, variable declaration and assignment, and novel syntax for quantum circuit generation and synthesis. Our approach enables an optimizing compiler for OpenQASM that compiles to the LLVM machine-level IR adherent to the recently introduced quantum intermediate representation (QIR) specification.\(^\text{1}\) Moreover, this approach need not be limited to OpenQASM—the implementation pattern shown in this work can serve as a robust mechanism for further quantum language compiler prototyping and deployment. The work presented here puts forward the requisite infrastructure for quantum language expression and LLVM IR generation, leaving future language compiler implementations as a matter of providing the mapping of a language abstract syntax tree (AST) to our quantum MLIR extension (via another tool for language recognition (ANTLR),\(^\text{14}\) for instance). Language lowering to executable code is then readily available.

We integrate our approach with the \texttt{qcor} compiler platform\(^\text{10}\) (note we use \texttt{QCOR} to denote the language extension specification and \texttt{qcor} for the compiler implementation). \texttt{qcor} enables single-source quantum–classical programming in both C++ and Python, promoting an ahead-of-time C++ compiler executable and just-in-time compilation infrastructure for performant quantum–classical code generation and execution. This work extends the \texttt{qcor} executable to standalone

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**FIGURE 1.** QCOR’s MLIR-based compilation stack for CPU-QPU heterogeneous computing. Each quantum programming language is processed by a dedicated parser that produces the AST of the input source code. AST of different source languages is all mapped to an MLIR representation expressed in the QCOR quantum dialect and built-in standard, affine, and SCF dialects. This MLIR representation is progressively (multistage) transformed (optimization and dialect conversion/lowering) until only operations in the LLVM dialect remain, i.e., quantum operations are converted to LLVM function calls adhering to the QIR specification. This guarantees that the final binary executable is compatible with any QIR-conformed runtime implementations provided at link time, such as \texttt{qcor} runtime supporting both remotely hosted (NISQ) and tightly coupled (FTQO) execution models.
OpenQASM source files, and enables their compilation and execution in a retargetable (quantum hardware-agnostic) fashion.

**BACKGROUND**

Figure 1 demonstrates the hierarchy of layers underlying our compiler architecture. Ultimately, we take quantum–classical languages down to an MLIR representation before emitting standard object code via lowering to the LLVM IR (we leverage the LLVM ecosystem of executables to map an IR bytecode representation to assembly and executable code). Here we seek to provide necessary background on the QIR specification, the MLIR framework, and the qcor compiler front-end and quantum runtime library to set up the presentation of the rest of the compiler architecture.

**Quantum Intermediate Representation**

Recent work has resulted in the development of a formal specification for a QIR embedded in the LLVM IR. This specification does not extend the LLVM IR with new instructions pertinent to quantum computing, instead, it expresses quantum specific operations as declared function calls on opaque data types. Function declarations and corresponding signatures are defined for quantum memory allocation and deallocation, individual qubit addressing, quantum instruction invocation on allocated qubits, and utility functions for array management, tuple creation, and callable invocation. By describing qubits, measurement results, and arrays as opaque types, and promoting function declarations over concrete implementations, the QIR specification promotes a flexible approach to quantum–classical compiler architecture and integration. The approach represents a novel target for language compilers—all of the LLVM toolchain becomes available, including runtime linking, compile time classical optimizations, and external language interoperability. Figure 2 demonstrates an LLVM IR code snippet adherent to the QIR specification for the generation of a GHZ maximally entangle state. Note the declaration of opaque Array and Qubit types (lines 1 and 2) and the externally declared QIR runtime functions (lines 4–10). These are left for implementation by appropriate QIR runtime libraries, affecting actual execution of quantum instructions, array handling (including arrays of Qubit instances), and data type actualization. The body of the code consists of standard LLVM instructions (bitcast, call, etc.) and calls to the declared QIR runtime functions. These functions are concretely provided at link time via the runtime library.

**Multilevel Intermediate Representation**

Moving up the IR abstraction hierarchy in Figure 1, recent developments in classical compilation research and development has resulted in the MLIR. The MLIR represents a modular and extensible approach to defining custom compiler IRs that can express a spectrum of language abstraction (language-level IR down to the machine-level LLVM IR). At its core, the framework puts forward the concept of a language dialect, which is composed of language-specific operations. These operations are the core abstraction unit in the MLIR, and they model a unique mapping of operands to return values, and can optionally carry a dictionary of compile-time metadata (attributes). Operands and return values are modeled as an mlir::Value type, which describes a computable, typed value, and its
The creation of dialects provides a mechanism for mapping language ASTs to a corresponding MLIR operation tree composed of language-dialect-specific operations alongside other utility dialect operations (standard function calls, memory references and allocation, for loops, conditional statements, etc.). Moreover, the framework puts forward a general progressive lowering capability—incremental translation of higher dialect operations to lower level dialect operations. This enables one to define custom translations from operations in language-level dialects to operations in a machine-level dialect, such as the LLVM IR. This infrastructure and corresponding workflow provide a flexible architecture for the development of compilation pathways taking language-level syntax trees down to a machine-level IR, such as the LLVM.

We want to note the novel utility of the MLIR for quantum–classical computing. As shown in Ittah et al.’s work, the static single assignment (SSA) characteristic of the MLIR enables efficient dataflow analysis and pattern rewriting, which proves critical for quantum circuit optimization via use-define chain tracking of common patterns that can be optimized. Moreover, the MLIR provides a wealth of classical optimizations that can be used in tandem with quantum optimizations. Classical IR passes may enable new downstream quantum IR passes that lead to more efficient quantum–classical code generation. Leveraging the MLIR for quantum–classical IR expression is therefore critical in that enables one to build upon the wealth of classical compiler research and development, while incrementally introducing quantum expression and optimizations.

qcor provides C++ and Python language extensions for heterogeneous quantum–classical computing in an effort to promote native quantum kernel programming in a single-source context. Critically, qcor puts forward a compiler runtime library that enables quantum program execution in a multimodal, retargetable fashion. The execution model enables two mode types of quantum instruction invocation—nisq and ftqc modes (see QCOR runtime linkage in Figure 1). nisq mode supports runtime-level quantum instruction queueing and flushing upon exit of a quantum kernel function, implying a full quantum circuit submission on a remotely hosted quantum computer. ftqc mode models a tightly coupled CPU–QPU integration model, and quantum instructions are instead streamed as they are invoked, enabling features like fast-feedback on qubit measurement results. The qcor runtime ultimately delegates to the XACC framework, and supports remote execution on IBM, Rigetti, IonQ, and Honeywell quantum processors, and has support for various simulators for the ftqc mode of execution. It is this runtime that plays a critical role in this work, as it provides a target for our QIR runtime library implementation. Moreover, we have provided an entrypoint to OpenQASM compilation natively as part of the qcor command line executable.

EXTENDING OpenQASM 3

OpenQASM version 3 has recently been put forward as a formal specification, and a extended Bachus–Naur form description of the language has been made public as an ANTLR grammar file. This language departs from the previous version (version 2.0) in the introduction of classical control flow and variable declarations, making version 3 much more friendly to hybrid quantum–classical programming. The language provides standard quantum instruction calls, but enables more complex quantum circuit synthesis via ctrl, adj, and pow quantum gate modifiers. Standard while and range-based for loops are also allowed, as well as the conditional if–else block.

WHILE OUR WORK SEEKS TO ENSURE THAT OUR COMPILER IMPLEMENTATION IS FULLY COMPATIBLE WITH THE BASE GRAMMAR SPECIFICATION FOR OpenQASM, WE ALSO ARE IN A UNIQUE POSITION TO ENHANCE IT WITH FEATURES PERTINENT TO THE QCOR COMPILER PLATFORM AND ITS USER BASE.

While our work seeks to ensure that our compiler implementation is fully compatible with the base grammar specification for OpenQASM, we also are in a unique position to enhance it with features pertinent to the qcor compiler platform and its user base. We envision the language and compiler presented in this work as a novel language extension for the qcor quantum kernel programming model, i.e., enabling users of qcor to program quantum kernels using our extended OpenQASM language. We seek extensions that (while remaining backwards compatible) enable a more C-like syntax, C-like primitive type declarations, and common quantum programming patterns already present in the
qcor language. To start, we have extended the grammar to provide familiar typedefs for 32- and 64-bit integers and floats. Specifically, we parse int as int[32], int64_t as int[64], float as float[32], and double as float[64]. We have also updated the grammar and implemented the parser to handle both range-based C-like for statements as well as the usual for statement with initializer, conditional expression, and iteration expression. Finally, we see an opportunity to enable syntax and semantics for specific compile-time optimizations. We have updated the OpenQASM grammar with support for the ubiquitous compute-action-uncompute pattern. Given the common pattern \( W = UVU^\dagger \), the new syntax enables one to express \( U \) and \( V \) as the code in the compute and action scopes, respectively, and the compiler auto generates the \( U^\dagger \) code after application of the compute, action segments. This is demonstrated in Figure 3(a) (addition to OpenQASM grammar) and (b) OpenQASM code leveraging the compute-action statement.

![Figure 3](image_url)

**FIGURE 3.** OpenQASM language extension for compute-action-uncompute pattern. (a) Compute-action ANTLR grammar addition, (b) OpenQASM code leveraging the compute-action statement.

**Symbol Table**

The symbol table is the data structure used by the compiler to cache information about each observed symbol (e.g., variable name, its type, its constness, etc.). Since OpenQASM allows for local variables, the symbol table becomes critical for tracking metadata about the variable symbol and its subsequent use. In other words, when processing each statement, the compiler, via the symbol table, is aware of the context of all visible symbols, i.e., those from this scope and those above, to perform proper name lookup. Therefore, the symbol table provides a mechanism to validate various semantic errors, such as illegal operations for a specific variable type or referring to out-of-scope variables, which could not be detected by syntactic considerations.

We have implemented a symbol table that is composed of an array of scope-indexed hash maps. Each map is a lookup table from variable name to the corresponding MLIR `mlir::Value` instance representing the variable. Name lookup is performed from the current scope upward (to parent scopes) to find the first match, i.e., the one in the nearest parent scope. Another utility of the symbol table is the compile-time evaluation of constant expressions. OpenQASM supports constant integer and floating-point variable declarations (via the `const` keyword). The symbol table tracks these constant values and provides a utility to evaluate simple math expressions\(^a\) involving these constants at compile time, if possible.

Critically, the compiler relies on the symbol table to track qubit use-define chains for quantum instruction operations (typical quantum gate invocations). We have designed our quantum instruction operation in the quantum MLIR dialect extension to adhere to

\(^a\)Using the C++ Mathematical Expression Toolkit (exprtk) Library.
the value semantics representation first described in Ittah et al.’s work, wherein quantum operations consume one or many qubit mlir::Value instances and produce one or many new mlir::Value instances as operation return types. Using the underlying pointer to the MLIR variable (mlir::Value) as the lookup key, the symbol table replaces input qubit operands with the newly created output mlir::Value. Therefore, the OpenQASM source code is compiled into the MLIR representation with explicit use-deﬁne chains for qubits amendable to compile-time optimization techniques similar to the DAG representation of quantum circuits.

ANTLR Parser

Our compiler implementation leverages the another tool for language recognition (ANTLR) toolchain to generate the compiler frontend, as depicted in Figure 4. With our extended OpenQASM grammar as input, ANTLR generates the corresponding lexers and parser utilities capable of scanning and parsing source strings according to the provided grammar rules. The compiler frontend produces an AST representing the input source code against the set of syntactic rules in the grammar. For instance, a valid OpenQASM loop (matching a syntax rule named loopStatement) will be parsed into a LoopStatementContext AST node along with all nested subnodes, e.g., the loop termination conditions and the loop body. ANTLR also generates a base AST visitor interface for each grammar file, which includes all possible AST node types that the parser may produce. The AST visitor is the mechanism we leverage to transform the raw OpenQASM syntax tree into the MLIR representation as we will discuss in the next section.

While processing the input source, the parser may throw exceptions indicating syntactic or semantic errors. The compiler implements the ANTLR BaseErrorListener interface (see Figure 4) to catch these potential issues and report them to users with detailed information, such as the location of offending characters.

Visitor Handlers

Once the valid OpenQASM source has been transformed into the ANTLR AST, the compiler traverses each node in the AST in a depth-first manner producing the equivalent MLIR tree using the standard (operations for classical control flow and memory references), afﬁne (operations for looping), and quantum dialects (our contribution modeling quantum operations). Table 1 summarized OpenQASM-MLIR rewrite patterns for important OpenQASM constructs.

In particular, quantum types (qubit and qreg) and classical types (boolean, variable-width integer or ﬂoating-point numbers, and arrays) are mapped to QIR types (Qubit and Array) or memory-referenced (mem-ref) MLIR Standard dialect types (e.g., i1 for boolean bits, i8 for 8-bit integers, etc.). Classical math operations are converted to the corresponding instructions from the MLIR Standard dialect, such as addi or cmpi for integer addition or comparison, respectively. Importantly, OpenQASM for loops are transformed into an AffineForOp (MLIR afﬁne dialect) amenable to future classical optimization passes, such as loop unrolling.

Intrinsic quantum gates are converted to value-semantics quantum operations [static single assignment form (SSA)] of the quantum dialect, as shown in Table 1. As described in the “Symbol Table” section, we use the symbol table to track the qubit operands (as opaque mlir::Value pointers) and replace them with the new values created by each value-semantics quantum gate operation. In other words, each qubit SSA variable (shown as %k in Table 1) will only be assigned and used once, thus allowing us to trace gate operations on each qubit line. This is to explicitly deﬁne the use-deﬁne chains, which we can leverage in downstream quantum optimizations.
Another key feature of OpenQASM is the ability to express quantum gate modifiers (e.g., controlled or adjoint) for both intrinsic gates and subroutines. Our compiler implementation takes a pragmatic approach by rewriting modifiers into scoped regions with dedicated MLIR marker operations, as shown in Table 1. These operations are effectively no-ops, but indicate to the runtime that the following region of quantum operations is to be treated as a modifier. 

### Table 1. Conversion of OpenQASM constructs to MLIR.

| Construct Type | OpenQASM                                                                 | MLIR                                                                 |
|---------------|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| Quantum Types |                                                                         |                                                                      |
| Qubit Register| `qubit qubit_array[20];`                                                   | `q0 = q.galloc(20); (name = qubit_array) : !quantum.Array`           |
| Classical Types|                                                                         |                                                                      |
| Bits          | `bit[20] bit_array;`                                                      | `q0 = alloca() : memref<20x1I>`                                     |
| Integers      | `int[16] short_int;`                                                     | `q0 = alloca() : memref<16I>`                                       |
| Floating point numbers | `float[32] np_float;`                                                | `q0 = alloca() : memref<f32>`                                       |
| Global Constants | `const shots = 1024;`                                             | `global_memref "private" constant $shots : memref<16I> = dense<1024>` |
| Quantum Instructions |                                                                         |                                                                      |
| Gates         | `ry(theta) q;`                                                          | `q4 = qsv.ry($%2, %3) : !quantum.Qubit`                              |
| Measurements  | `b = measure q;`                                                        | `q7 = q.nr($%6) : !quantum.Result`                                  |
|               |                                                                         | `q9 = q.resultCast($%7) : i1`                                        |
|               |                                                                         | `store $9, %0[] : memref<i1>`                                       |
| Classical Operations |                                                                         |                                                                      |
| A hack        | `a += 4;`                                                               | `%c4_i64 = constant 4 : i64`                                        |
|               |                                                                         | `%1 = load %0[] : memref<i64>`                                       |
|               |                                                                         | `%2 = add %1, %c4_i64 : i64`                                         |
|               |                                                                         | `store %2, %0[] : memref<i64>`                                       |
| Branching     | `if [1 == 5] {...}`                                                     | `%c5_i64 = constant 5 : i64`                                        |
|               |                                                                         | `%1 = load %0[] : memref<i64>`                                       |
|               |                                                                         | `%2 = cmpi "eq", %1, %c5_i64 : i64`                                 |
|               |                                                                         | `cond br %2, "%bb1", "%bb2"                                        |
|               |                                                                         | `bb1: // pred: "bb0"`                                                |
|               |                                                                         | `bb2: // 2 preds: "bb0", "%bb1"`                                   |
| Looping       | `for i in [0:10] {...}`                                                 | `affine.for %arg6 = affine_map<0> -> (0) to -> affine_map<0> -> (0) : () {...)` |
|               |                                                                         | Note: %0: memref<i64> (represents a variable)                         |
| Subroutines   | `def foo(float[64]:theta); qubit[2]:q { ... }`                           | `func @foo(float[64], float[64]:theta) -> (float[64])` |
|               |                                                                         | Note: %5: index and %7: index represent the constant values of 10 and 0, respectively. |
| Modifiers     |                                                                         |                                                                      |
| Adjoint       | `inv 0 phase(pi) q;`                                                    | `q.adj_region ( ... `                                           |
|               |                                                                         | `q2 = qsv.phase(%1, %0) : !quantum.Qubit)`                           |
| Controlled    | `ctrl 0 oracle q[0], q[1];`                                             | `q.ctrl_region ( ... `                                            |
|               |                                                                         | `q3 = call @oracle(%0) : (!quantum.Qubit) -> !quantum.Qubit)`         |
| Power         | `pow(8) & foo q;`                                                       | `q.pow_u_region ( ... `                                            |
|               |                                                                         | `q#_i64 = constant 8 : i64`                                         |
|               |                                                                         | `q2 = call @pow(%0) : (!quantum.Qubit) -> !quantum.Qubit)`            |
|               |                                                                         | `pow = %c8_i64`                                                      |
| Aliasing      |                                                                         |                                                                      |
| Slicing       | `let slice = reg[0:2:12];`                                              | `%1 = q.qarray_slice(%0, %c0_i64, %c2_i64, %c12_i64) : !quantum.Array` |
|               |                                                                         | `%2 = q.qarray_concat (%0, %1) : !quantum.Array`                      |
| Concatenation | `let concat = reg1 || reg2;`                                            |                                                                      |
operations is to be handled differently. For example, for the ctrl marker (q.ctrl_region), the operations within that region should be processed to synthesize the controlled version of that composite operation. We preserve the high-level semantics of these modifiers at both the MLIR and latter LLVM IR levels (see the “Dialect Conversion and Lowering” section) rather than trying to perform compile-time gate synthesis. Ultimately, the evaluation and synthesis of these modifier-enclosed blocks will be performed by QIR-compatible runtime implementation.

To handle the nested, recursive nature of the OpenQASM syntax tree, the compiler uses a multilayer visiting strategy whereby a standalone visitor-like utility, named qasm3_expression_generator, is provided to traverse and process subexpression nodes in-place, if necessary. To give an example, when visiting a for loop with a math expression as its upper bound, the main AST visitor would use this qasm3_expression_generator to handle this subexpression (converting the math expression to a MLIR equivalent) and then take the resulting value (as a mlir::Value) to construct the current MLIR for loop.

Progressive Lowering
After visiting all the ANTLR AST nodes representing the input OpenQASM program, the compiler has constructed an MLIR code in the quantum, affine, standard, and built-in dialects. As depicted in Figure 5, this is the first stage of a progressive, multistage IR transformation and lowering pipeline that produces an optimized executable.

Next, we perform a set of optimization passes at the MLIR level whereby control flow constructs (e.g., those from the affine dialect) and the SSA form of quantum instructions in the quantum dialect are suitable for static optimization procedures. The optimized MLIR code is lowered to the LLVM dialect via the MLIR ConversionPattern utility. At this point, all quantum-related operations have been lowered to QIR functions. The final lowering to LLVM IR and any built-in

FIGURE 5. Compilation pipeline: The ANTLR-based frontend parses the OpenQASM source string into an AST data structure. By processing (visiting) the AST, we generate an MLIR representation using a couple of dialects, most importantly, our quantum dialect. A set of optimization passes can be applied at this stage to simplify the MLIR tree before it is lowered to the LLVM dialect. At this stage, the IR tree only contains valid LLVM instructions including QIR-adherent function calls and types. Standard LLVM optimization can be applied when the LLVM dialect is lowered to bitcode, e.g., the -O3 LLVM optimization flag. Finally, the LLVM IR bitcode is compiled to binary executable by linking in a compatible QIR runtime implementation.

AFTER VISITING ALL THE ANTLR AST NODES REPRESENTING THE INPUT OpenQASM PROGRAM, THE COMPILER HAS CONSTRUCTED AN MLIR CODE IN THE QUANTUM, AFFINE, STANDARD, AND BUILT-IN DIALECTS.

FIGURE 6. Optimization pass pipeline. Optimization passes simplifying quantum gate operations are repeated a set number of times.
LLVM optimizations (e.g., `O3` optimization) are provided by the MLIR–LLVM infrastructure, producing binary executables targeting the QIR runtime along with the classical compute ISA (e.g., x86/Arm/OpenPC depending on the target platform).

**Optimization Passes**

Figure 6 illustrates the MLIR-level optimization pipeline that we have implemented in the OpenQASM compiler.

Specifically, we combine optimization techniques from both classical and quantum programming, such as function inlining, loop unrolling, and various quantum circuit optimization procedures. Table 2 lists the quantum optimization passes that we have implemented for the MLIR operations in `OpenQASM`.

**TABLE 2.** List of MLIR optimization passes.

| Pass name                      | Descriptions                                                                 |
|--------------------------------|-----------------------------------------------------------------------------|
| Identity pair removal          | Simplify or remove redundant quantum instructions. For example, this pass removes any gates immediately followed by their adjoints, such as pairs of X–X, T–T, or CNOT–CNOT gates on the same qubits. Repeated qubit reset instructions are also simplified. |
| Rotation merging               | Combine consecutive mergable quantum instructions, e.g., Z and Rz(θ), Rx(θ₁), Rx(θ₂), etc. |
| Gate sequence simplification   | Find a sequence of consecutive compile-time constant gates and simplify if possible, i.e., resynthesize to fewer gates. For example, H–T–H gate sequence can be simplified to Rx(π/4). |
| Qubit extract lifting          | Merge duplicate qubit extracts from registers with compile-time constant indices. This pass also unifies the SSA use-define chain after loop unrolling (loop induction variable as qubit array index) and function inlining. |
| Gate permutation               | Permute gates that are commutative, e.g., Rz on the control qubit of a CNOT gate. Despite no immediate benefit (no gate count reduction), this pass might provide optimization opportunities for others, such as rotation merging. |
| Constant propagation          | Propagate global constants, e.g., constant integer values as loop counts or constant floating points as rotation angles. |
| Dead code elimination (DCE)    | Eliminate unused operations (dead code). For example, qreg allocation whose result is never used can be eliminated. These dead values may emerge as a result of other passes. |

**Figure 7.** MLIR optimization example. The input (a) OpenQASM source code is first compiled into the (b) MLIR representation, which is then processed by a sequence of optimization passes. After the call to `foo` (b, line 2) is inclined, (c) the back-to-back CNOT pattern emerges; thus, both gates are removed by the (d) identity pair removal pass. Finally, the (e) DCE pass eliminates the redundant qubit array allocation, constant value declarations, and qubit extract calls since they have no further use.
our quantum dialect. Inlining and loop unrolling are built-in MLIR passes for the standard and affine dialects, respectively.

The pseudocode in Algorithm 1 illustrates a typical MLIR optimization pass based on dataflow analysis. Specifically, we show the procedure to perform quantum gate merging on the MLIR AST tree. By adhering to value-semantics for the quantum operations, we are able to follow the use-define chain of each quantum instruction (shown as the User map in Algorithm 1). With the SSA dataflow information, we can query the next quantum operation on the qubit line and check whether a gate-merge opportunity exists. For illustration purposes, we depict the gate merging procedure as two black-box functions, CanMerge and Merge, implementing checking and gate generation procedures. The new injected gate operation will have its input and output SSA values bridging those two original instructions (lines 10 and 11 in Algorithm 1). Each optimization pass operating on the MLIR operation tree maintains the SSA value chain as they transform the IR.

Algorithm 1. Gate merging optimization

| Vars: |
|---|
| † ops : [VSOp] (Sequence of value semantics ops) |
| † Users: VSOp \(\rightarrow\) [VSOp] (use-define trace mechanism) |
| † CanMerge: (VSOp, VSOp) \(\rightarrow\) \(\mathbb{I}\) (Mergeable check) |
| † Merge: (VSOp, VSOp) \(\rightarrow\) VSOp (Create merge op) |

**Gate Merging:**

1. dead_ops : [VSOp] \(\leftarrow\) []
2. for op \(\in\) ops do
3. if op \(\in\) dead_ops then
4. Skip to next op
5. end if
6. if Length(Users(op)) \(=\) 1 then
7. next_op \(\leftarrow\) Users(op)[0]
8. if CanMerge(op, next_op) then
9. merged_op \(\leftarrow\) Merge(op, next_op)
10. merged_op.input \(\leftarrow\) op.input
11. merged_op.output \(\leftarrow\) next_op.output
12. Add merged_op to IR tree
13. Append op and next_op to dead_ops
14. end if
15. end if
16. end for
17. for op \(\in\) dead_ops do
18. Erase op from IR tree
19. end for

We also want to note that this optimization procedure, as well as others listed in Table 2, is most effective when the AST is a flat linear region whereby the use-define chain is uninterrupted (e.g., due to subroutine calls or loops). Therefore, it is crucial to have loop unrolling and function inlining passes applied beforehand, as shown in Figure 6. In this pass pipeline, some passes, especially those performing quantum circuit optimization, are applied multiple times in a loop to make sure that we can pick up new optimizing patterns that emerged thanks to the code rewrite of previous passes.

In Figure 7, we demonstrate the MLIR transformation along the optimization pipeline for a simple OpenQASM source code [see Figure 7(a)]. This code contains a subroutine definition and later invocation, which is compiled to the MLIR CallOp [line 2 in Figure 7(b)]. This call is then inlined [see Figure 7(c), lines 4–6], resulting in a \texttt{NOT} identity pair, which is removed by the identity pair removal pass [see Figure 7(d)]. What is left after this step is a sequence of unused operations, such as extracting qubit addresses and the 	exttt{reg} allocation itself. These are all dead code, hence removed by the final DCE pass, as shown in Figure 7(e).

**Dialect Conversion and Lowering**

After simplifying the MLIR tree with optimization passes, such as those listed in Table 2, the compiler will lower the MLIR representation to LLVM progressively, as depicted in Figure 5. This lowering procedure is similar to the one described in McCaskey and Nguyen’s work\(^6\) for OpenQASM 2 compilation. We implemented a collection of \texttt{mlir::ConversionPattern} to perform the conversion from quantum dialect to the LLVM dialect targeting the QIR specification.

As compared to the work in McCaskey and Nguyen’s work\(^6\), the lowering pipeline of the qcor compiler has been enhanced with 1) dialect conversion from affine to LLVM branch-based CFG (control flow graph) representation and 2) conversion pattern implementations for new quantum dialect operations. The first one stems from the fact that we utilize operations from the affine dialect to handle control flows (e.g., for loops) in OpenQASM. The latter involves lowering procedures for new quantum dialect operations for gate modifiers (see Table 1) as well as the new quantum value semantics instruction. MLIR modifier-marked regions (\texttt{ctrl}, \texttt{inv}, or \texttt{pow}) are converted to the calls to corresponding quantum runtime functions at the beginning and the end of the scoped block. To lower the value-semantics quantum operations (MLIR quantum dialect) to memory-semantics LLVM QIR calls, the qubit SSA variables are mapped back to their root variable (in the use-define chain) by
propagating the mlir::Value of input qubit operands to the corresponding outputs.

QIR Implementation and Linking
The last stage of the compilation workflow, as shown in Figure 5, involves the compilation of LLVM IR bytecode into a binary object containing QIR function calls, that needs to be linked to a valid QIR runtime implementation to form an executable. As described in McCaskey and Nguyen’s work, qcor provides a QIR runtime library implementation backed by the XACC framework.

Since quantum value-semantics operations are converted to memory-semantics function calls [e.g., void __quantum_qis_INSTNAME(qubit*, ...)] during the lowering stage, they are compatible with the existing QIR intrinsic quantum gates in the runtime. Key extensions to the QIR runtime to support OpenQASM are the region marker functions to implement gate modifier concepts, such as controlled (ctrl) or adjoint (inv). Specifically, when a quantum gate or subroutine is subjected to a modifier directive, the compiler injects the corresponding runtime functions before and after the modified operation. For example, __quantum_rt_start_adj_u_region and __quantum_rt_end_adj_u_region are functions to denote a region of code whereby the inverse (adjoint) of the collected quantum sequence generated within should be applied. Once again, we take a pragmatic approach in implementing the gate modifier feature of the OpenQASM language by delegating the modified circuit realization to the runtime. By invoking the wrapped code region at runtime in a special instruction collection mode, we can retrieve the flattened sequence of gates and thus construct the corresponding modified circuit (e.g., adjoint or controlled) for backend execution.

Finally, the QIR runtime environment can be further specialized via compilation flags or executable invocation arguments. For instance, specific hardware or simulator backend (qpu) can be selected, and the quantum runtime can be configured to run in a tightly coupled execution mode (simulator-only) whereby the dynamical measurement-controlled branching is fully supported.

DEMONSTRATION
In this section, we demonstrate the utility and performance of an MLIR-based compiler. We present a typical OpenQASM programming, compilation, and execution workflow using the qcor infrastructure. The compilation speed is benchmarked against a variety of comparable quantum compilers. Finally, we provide an example showing extensions to the OpenQASM language provided by qcor.

**Compilation and Execution Workflow**
Figure 8 shows an OpenQASM source code to compute the expectation value of Pauli operators ($\sigma_x\sigma_y\sigma_z$) after a state-preparation circuit (ansatz).

```
OPENQASM 3;
include "stdgates.inc";
const shots = 1024;
// State-preparation:
def ansatz(float[64]:theta) qubit[2]: q {
  x q[0];
  ry(theta) q[1];
  cx q[1], q[0];
}
def compute(float[64]:theta) qubit[2]: q ->
  float[64] {
    bit first, second;
    float[64] num_parity_one = 0.0;
    float[64] result;
    for i in [0:shots] {
      ansatz(theta) q;
      // Change measurement basis
      h q;
      // Measure
      first = measure q[0];
      second = measure q[1];
      if (first != second) {
        num_parity_one += 1.0;
      }
      // Reset
      reset q;
    }
    // Compute expectation value
    result = (shots - num_parity_one) / shots -
              num_parity_one / shots;
    return result;
  }
float[64] theta, exp_val;
qubit qq[2];
// Try a theta value:
theta = 0.123;
exp_val = compute(theta) qq;
print("Avg <X|X> = ", exp_val);
```

**FIGURE 8.** OpenQASM example: Compute Pauli expectation ($\sigma_x\sigma_y\sigma_z$) after a state-preparation circuit (ansatz).

We anticipate that quantum hardware providers will support this dynamical runtime model in the near future as OpenQASM becomes more mature and widely adopted.
A feature that we want to highlight is the fact that Pauli expectation accumulation is explicitly expressed as a for loop (lines 16–28). Note the \texttt{quantum instruc-}

\begin{verbatim}
func @compute(temp0: f64, temp1: iquant.Array)
  -> f64 {
    ... 
    br "bbl"  // 2 preds: "bbl", "bb5"
    "bbl": // 2 preds: "bbl", "bb5"
    %6 = cmpi "sl", %5, %c:224.164 : i64
    cond_br %6, "bb3", "bb3"
    "bb2": // pred: "bb1"
    %7 = q.extract(temp0, %c:164) :
    → @quantum.Qubit
    %8 = qvz.x(%7) : !quantum.Qubit
    %9 = q.extract(temp0, %c:164) :
    → @quantum.Qubit
    %10 = qvz.y(%8, %arg0) : !quantum.Qubit
    %11 = qvz.x(%10, %arg1) : !quantum.Qubit, → @quantum.Qubit
    ... 
    %23 = cmpi "ne", %21, %22 : i1
    cond_br %23, "bb4", "bb5"
    "bb5": // pred: "bb1"
    ... 
    %29 = subf %27, %26 : f64
    ... 
    return %29 : f64
    "bb6": // pred: "bb2"
    %30 = load %21 : memref<f64>
    %41 = addf %40, %test0 : f64
    store %41, %21 : memref<f64>
    br "bbl"
    "bb5": // 2 preds: "bb2", "bb4"
    %42 = qvz.reset(%14) : @quantum.Qubit
    %43 = qvz.reset(%16) : @quantum.Qubit
    %44 = load %44 : memref<f64>
    %45 = addi %44, %c:164 : i64
    store %45, %44 : memref%i64
    br "bbl"
\end{verbatim}

A feature that we want to highlight is the fact that Pauli expectation accumulation is explicitly expressed as a for loop (lines 16–28). Note the `quantum instruc-

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure9.png}
\caption{Truncated MLIR representation of the OpenQASM program in Figure 8. Here, we only show a simplified MLIR printout of the core deuteron function whereby most of the code has been omitted for clarity. High-level classical control flow constructs, such as the for loop and the if statement in Figure 8 are converted into LLVM-style CFG constructs and operations, such as blocks and branches. Thanks to MLIR-level optimization (see the “Optimization Passes” section), the \texttt{ansatz} subroutine in Figure 8 has been inlined into the deuteron body, as shown as \texttt{qvz.x, qvz.ry, and qvz.cx} operations. Arithmetic operations are translated to MLIR operations from the Standard dialect, such as \texttt{addf, subf, divf} (floating-point numbers) or \texttt{addi, and cmpi} (integers).}
\end{figure}

For the sake of presentation, we only keep the high-level structure of the MLIR printout (omitted regions are presented as ellipses).

The semantics of the OpenQASM source code is faithfully translated into the MLIR representation consisting of operations from our quantum dialect (e.g., quantum gates) and the standard dialect (e.g., branching and arithmetic instructions). We can now transform this high-level IR to executable code adhering to the QIR specification (see Figure 5). At the time of writing, the execution of this type of tightly coupled quantum–classical program, whereby measurement feedforward is required, is only applicable to simulator backends of qcor’s \texttt{QIR} compilation. We anticipate that quantum hardware providers will support this dynamical runtime model in the near future as OpenQASM becomes more mature and widely adopted. Importantly, in our workflow, the runtime implementation is linked in at the final phase of the compilation pipeline, thus could be provided interchangeably and dynamically to target different accelerator targets.
Compiler Performance

In this section, we benchmark (setup: Intel Xeon CPU E5-2698 v4 @ 2.20 GHz running Linux Debian 10 distribution) the compilation and resource estimation runtime of the OpenQASM compiler against a set of different quantum programming languages and frameworks, such as Q#, (Microsoft Quantum Development Kit 0.18.2107153439) Qiskit, (qiskit-terra 0.18.1) and tket. (pytket 0.13.0) We benchmark the total runtime required to generate and execute binary executables in the resource estimation mode, i.e., counting flattened quantum gates, because it provides a mechanism to compare statically compiled executables against Python-based interpreted scripts constructing the equivalent circuits.

In Figure 10, we plot the compile data for Trotter circuits simulating the generic Heisenberg Hamiltonian model of the form

$$H = -\hbar \sum_i (X_i \otimes Z_i + J_z X_i Z_i + 1).$$

The circuit is constructed by “for” loops over a fixed number of Trotter steps [steps = 100, step size ($dt$) = 0.01] with a variable number of qubits from 5 to 50. In other words, we construct the circuit representing the unitary

$$U = \prod_{i=1}^{100} \left( \prod_i \exp(-\hbar dt X_i) \prod_i \exp(-J_z dt Z_i Z_{i+1}) \right)$$

where each Pauli exponential term is converted to an equivalent gate-based subcircuit. These subcircuits are repeated at each time step to simulate the Trotterized evolution of the Heisenberg Hamiltonian.

Quantum programming languages, such as Q# and OpenQASM, preserve the loop construct in their IR representation, resulting in almost constant compilation time. We note that the number of qubits is a compile-time constant for both the Q# and OpenQASM cases. The compiler may choose to unroll these loops.

The compilation time of OpenQASM includes: 1) front-end parsing (ANTLR), 2) MLIR generation and optimization, 3) lowering to LLVM IR, 4) LLVM optimization, and
5) object code generation and linking. For Q#, we leverage the Microsoft Quantum Development Kit (QDK) to perform QIR LLVM generation, i.e., equivalent to steps 1–3 in our OpenQASM workflow. The QDK-generated LLVM IR is then optimized and linked with the qcor runtime similar to steps 4 and 5 using the standard LLVM toolchain.

The results in Figure 10 highlight the need for statically compiled quantum programming languages in order to describe large-scale programs. Imperative gate-by-gate construction of quantum circuits using scripting languages, despite its flexibility and ease of use, does come with a significant performance overhead. Importantly, our MLIR-based compiler for OpenQASM demonstrates improved performance compared to other compilers, such as Q#. It is worth noting that the Q# language is much more feature-rich than OpenQASM, therefore requiring a more elaborated frontend and build system. In particular, initial Q# to QIR generation accounts for the majority (80%–90%) of the total Q# compilation time in Figure 10. As of this writing, there are no other publicly available OpenQASM compilers that we can compare our implementation with.

Extensions for Optimal Code Generation

Here we demonstrate the utility of our proposed extensions to the OpenQASM grammar specification with regards to optimal quantum code generation. Specifically, we show how the compute-action syntax enables the compiler implementation to generate optimal quantum instruction sequences in the presence of a c\textit{trl} gate modifier. As stated in the “Extending OpenQASM 3” section, controlled operations on the \(W = U^{\dagger}V U\) pattern only require controls applied to the operations in \(V\). Via programmer intent—i.e., leveraging the custom compute \(\ldots\) action \(\ldots\) syntax—the compiler can optimally synthesize quantum instruction sequences adherent to this pattern.

Take the Heisenberg Hamiltonian and corresponding time evolution operator \(U\) in (1) and (2). In the context of the quantum phase estimation algorithm, if we seek a corresponding eigenvalue of \(U\) with respect to some eigenstate \(|\psi\rangle\), we will require the application of a series of controlled versions of \(U\).

Figure 11 shows an OpenQASM subroutine describing the trotter evolution in (2). The second nested for loop (lines 18–29) could be written manually as the sequence \(W = CX \otimes RZ(\theta) \otimes CX_1\), but by replacing it with a compute-action block, we give the compiler an opportunity for optimal instruction synthesis under application of a c\textit{trl} modifier. Specifically, we have implemented an ANTLR visitor handler that processes the compute-action source and adds the compute instructions, the action instructions, and the adjoint or reverse of the compute instructions to the MLIR tree. Moreover, for instructions that are not in the action block, the compiler marks the added instructions with a flag to indicate that they are part of the compute or uncompute block. At runtime, this information is used to optimally synthesize controlled versions of this block of code.

We benchmark the usage of compute-action versus manual programming of \(W\) and present the results in Figure 12. The results show the number of controlled operations (CRZ, CNOT) present in the compiled quantum program for the manual (commented lines 22–26) and compute-action (lines 17–21) cases. One can clearly see that via programmer intent, the compiler can optimally synthesize instruction sequences and improve on the resource utility of the compiled program. With this simple programming extension, programmers can pick up an order of magnitude in gate count reductions.

**CONCLUSION**

We have presented an optimizing ahead-of-time OpenQASM compiler built on the MLIR framework. Our approach lowers OpenQASM codes to the LLVM IR in a manner that is adherent to the QIR specification. We provide quantum circuit optimization passes at the MLIR level and leverage existing classical optimization passes present in both MLIR and LLVM. Our work extends the OpenQASM grammar with support for C-like constructs and the compute-action-uncompute pattern for efficient programming and compile-time optimizations. Targeting the QIR enables one to swap runtime library implementations enabling a write once run anywhere characteristic. We have provided a runtime library implementation of the QIR specification that is backed by the XACC quantum programming framework, thereby enabling OpenQASM compilation that targets quantum computers from IBM, Rigetti, Honeywell, IonQ, as well as simulators that scale from laptops to large-scale heterogeneous high performance computers, like Summit. Moving forward, our approach opens up the possibility of true language integration at the LLVM IR level. We envision a number of language approaches that map to the LLVM IR adherent to the QIR specification, and via simple runtime linking, enabling the integration of quantum language A with code from quantum language B. As of this writing, the integration of Q#, qcor C++, and OpenQASM is now possible. We also envision this work as an alternative mechanism for embedded C++ quantum kernels in qcor, departing from the existing Clang Syntax Handler source preprocessing. Future work will investigate true quantum language integration and compile-time embedding of MLIR-to-LLVM processing in the qcor C++ language extension.
Here, we list all the source codes used for the Trotter circuit benchmarking (see Figure 10). The number of qubits in the Q# and OpenQASM source codes represent a particular data point. We modify the number of qubits and recompile the source code for the benchmark.

**A.1 Qiskit Script**

```python
from qiskit.quantum_info import QasmSimulator
from qiskit.transpiler import PassManager
from qiskit.transpiler import PassManager
from qiskit.transpiler import PassManager

# define the circuit
q = qasm_simulator = QasmSimulator(backend=backend)

# define the parameters
N = 10
J = 1.0
J_x = 0.5
J_y = 0.0
J_z = 0.0

# define the Hamiltonian
H = J * qasm_simulator + J_x * qasm_simulator + J_y * qasm_simulator + J_z * qasm_simulator

# simulate the circuit
result = qasm_simulator.run(H, shots=1000, seed=42).result()

# print the results
print(result.get_counts(H))
```

**A.2 tket Script**

```python
import time

# define the circuit
q = QasmSimulator(backend=backend)

# define the parameters
N = 10
J = 1.0

# define the Hamiltonian
H = J * qasm_simulator + J_x * qasm_simulator + J_y * qasm_simulator + J_z * qasm_simulator

# simulate the circuit
result = qasm_simulator.run(H, shots=1000, seed=42).result()

# print the results
print(result.get_counts(H))
```

**A.3 Q# Source Code**

```qsharp
namespace Benchmark.Heisenberg {
    open Microsoft.Quantum.Intrinsic;
    open Microsoft.Quantum.Canon;
    open Microsoft.Quantum.Math;
    open Microsoft.Quantum.Convert;
    open Microsoft.Quantum.Arrays;
    open Microsoft.Quantum.Measurement;

    // In this example, we will show how to simulate the time evolution of a Heisenberg model. We pick arbitrary values for the X and J couplings and use trotterStepsPerDouble = Unit (1) to simulate the Trotter step.}

    // This determines the number of Trotter steps
    let trotterStepsPerDouble = Double; 1.0;
}
```

*COMPILING FOR ACCELERATORS*
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