Extending Python for Quantum-Classical Computing via Quantum Just-in-Time Compilation

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Python is a popular programming language known for its flexibility, usability, readability, and focus on developer productivity. The quantum software community has adopted Python on a number of large-scale efforts due to these characteristics, as well as the remote nature of near-term quantum processors. The use of Python has enabled quick prototyping for quantum code that directly benefits pertinent research and development efforts in quantum scientific computing. However, this rapid prototyping ability comes at the cost of future performant integration for tightly-coupled CPU-QPU architectures with fast-feedback. Here we present a language extension to Python that enables heterogeneous quantum-classical computing via a robust C++ infrastructure for quantum just-in-time (QJIT) compilation. Our work builds off the QCOR C++ language extension and compiler infrastructure to enable a single-source, quantum hardware-agnostic approach to quantum-classical computing that retains the performance required for tightly coupled CPU-QPU compute models. We detail this Pythonic extension, its programming model and underlying software architecture, and provide a robust set of examples to demonstrate the utility of our approach.

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1 INTRODUCTION
The availability of noisy quantum hardware has necessitated the concurrent advance of corresponding software and tooling for enabling remote programming, compilation, and execution. Vendors have put forward concrete, noisy implementations of superconducting, ion trap, and photonic quantum computers, and most have provided corresponding software frameworks for low-level circuit construction and remote execution over HTTP REST APIs. This concurrent hardware-software implementation strategy has resulted in a number of high-level scientific computing demonstrations pertinent to fields like nuclear physics, quantum chemistry, and machine learning [9, 11, 17, 19]. The software frameworks put forward over the past few years have primarily leveraged Python to provide a high-level language approach to quantum-classical programming [2, 8, 14, 16, 25]. The decision to use Python makes sense for near-term quantum-classical computing tasks for a number of reasons: (1) the remote nature of the CPU-QPU interaction...
removes any possibility of performance (therefore a less-performant language like Python suffices), (2) the wide availability of libraries for common tasks like network programming, (3) the experimental nature of near-term quantum processors necessitates the quick-prototyping capability provided by scripting, and (4) the grass-roots development of tutorials and teaching materials for quantum programming puts a strong focus on easy-to-learn scripting languages commonly taught in University computer science programs.

A consequence of the wealth of development activities coming from these separate vendor framework efforts has been the lack of a unified interface, a true integration platform, for near-term quantum computation at the Pythonic language level. A number of frameworks have moved toward an architectural model that enables backend injection via the development of pertinent subclasses, however, each framework is primarily focused on providing strong support for the hardware backend it was originally intended for. Programmers, therefore, are forced to switch frameworks - learn new data structures and models - every time they want to program a different quantum computer, if they desire to get the most out of the feature set provided by the framework. This has a large effect on algorithmic and benchmarking research activities that require the ability to quickly prototype algorithms and applications and compare execution across a variety of near-term QPUs.

Here we present a programming model that builds upon the qcor C++ language extension [21, 23] to provide a unified interface and integration platform for quantum-classical computing at the Python language level. Specifically, we provide a language extension to Python that enables a just-in-time (JIT), retargetable compiler for quantum-classical Python scripts that wholly delegates to a performant C++ infrastructure. Our approach allows programmers to write quantum-classical codes at a high-level in Python in a way that supports quick prototyping, library integration, and dynamic typing in a write-once, run-anywhere manner. Our approach is truly hardware-agnostic, with backend support from IBM, Rigetti, Honeywell, and others, as well as Summit-scale quantum circuit simulation technologies.

This paper is structured as follows: first we provide relevant background on the qcor C++ language extension and compiler infrastructure. We then detail how we extend that infrastructure for Pythonic quantum kernel parsing and compilation in C++. Next we provide a detailed exposition of the qcor just-in-time compilation infrastructure, enabling the compilation and execution of quantum kernel strings at runtime. Finally, with this background in place, we detail how we provide our Pythonic language extension (quantum kernels in Python) via delegation to this C++ JIT infrastructure. We end with a demonstration detailing pertinent examples of the utility of this work.

2 QCOR

Recently, a language extension specification [21] has been proposed for heterogeneous quantum-classical computing that seeks to enable a single-source, accelerated-node programming model by leveraging language-native functions to express quantum code (kernels) intended for compilation and execution on a quantum co-processor. This specification, QCOR, has recently been implemented as an extension to C++ via a compiler infrastructure called qcor [23]. The qcor compiler enables the expression of quantum kernels as standalone, annotated functions in C++ and compiles these hybrid quantum-classical source files in a manner that enables quantum backend retargetability. qcor achieves this functionality by extending key plugin interfaces in Clang that enable quantum kernel language parsing and syntax handling at compile-time (after preprocessing, before abstract-syntax-tree generation). The Clang SyntaxHandler extension point [10] provides implementors with an opportunity to analyze invalid domain specific language code and map it to appropriate, valid C++ API calls. qcor puts forward a SyntaxHandler that maps invalid quantum code to valid API calls that target the XACC quantum-classical programming framework [18]. In this way, the qcor compiler represents the integration of classical compiler software technologies with the XACC programming model and concrete implementation for gate-model quantum-classical computing. XACC is leveraged by qcor for its quantum intermediate representation (IR), IR transformation infrastructure, backend quantum co-processor extensibility, and language parsing capabilities.
Moreover, the qcor SyntaxHandler implementation is further decomposed into a unique TokenHandler interface which is implemented for new quantum domain specific languages, thereby enabling extensible quantum language expression and utility within quantum kernel function bodies. The goal of a TokenHandler sub-type is to analyze incoming observed Clang Tokens and provide valid C++ code as a replacement that affects construction of the XACC IR and its execution on the desired backend quantum co-processor. qcor currently has TokenCollector implementations that enable kernel programming using the XASM and OpenQASM 2.0 assembly dialects, as well as a unitary matrix decomposition language for high-level quantum program expression. As an extension point to the qcor compiler platform, developers are free to enable quantum code expression in a way that best suits the situation at hand. For this work - extending Python with support for quantum kernel expression - we seek a TokenCollector implementation that will parse Pytonic quantum assembly expressions with support for typical Pytonic control flow constructs like for and if.

The following sections will detail how we leverage the TokenCollector to enable quantum kernel programming in C++ using a Pytonic version of the XASM dialect. With this in place, we detail how to leverage these expressions via just-in-time compilation of qcor quantum kernels (QJIT). Finally, we show how this QJIT infrastructure is leveraged from Python to enable high-level Pytonic quantum kernel expression and utility via standard Python function decorators.

2.1 New qcor C++ Language Features

Before diving into the specifics of our Python language extension for quantum computing based on qcor, it is pertinent to mention new features that have made it into the C++ language extension since the publication of [23]. We note these to raise awareness of them, but also because a goal of the Python extension is to support all features that the C++ extension supports. The added features described in this section are also provided by the Pytonic extension described by this work.

2.1.1 Compute - Action - Uncompute Programming Pattern. A common pattern in quantum computing is the $U - V - U^\dagger$ sequence [12], with unitary matrices $U$ and $V$. It is often referred to as the compute-action-uncompute pattern due to the cancellation effect of $U^\dagger$. For example, quantum circuits implementing reversible logic [4] usually have this structure. A recent enhancement to the qcor compiler frontend and its runtime allows users to capture this specific pattern by introducing the compute and action keywords. The language expects a brace-enclosed sub-kernel, e.g., quantum gates, after each of these two keywords. The uncompute circuit, i.e., the adjoint of the compute gate sequence, is appended automatically after the action block by the compiler. Once the compiler detects this pattern, it marks the compute sub-circuit segment by injecting calls to the internal qcor runtime functions at the beginning and the end of the sub-circuit. Thanks to these markers, the qcor runtime will be able to collect the gate sequence representing the compute $U$ matrix and then append its conjugate after the action segment.

In addition to improving the expressibility of the language, this compute-action construct also benefits controlled circuit generation. Due to the cancellation effect of the $U - U^\dagger$ pair, we do not need to add control qubits to these two segments but just the middle action $V$ segment. Therefore, the resulting controlled circuit is potentially much shorter than a naive gate-by-gate transformation without this high-level structural meta information.

2.1.2 Callable Quantum Kernel Arguments and Lambda Expressions. A major component of the qcor compiler platform is its standard library implementation providing commonly used subroutines, such as Grover’s algorithm, quantum Fourier transforms, error correction procedures, etc. To develop generic, library-oriented kernels, it is imperative to be able to pass quantum kernels as arguments to other kernels. To address this requirement, we introduce a new core concept into qcor — the KernelSignature, which is very similar to the QuantumKernel class [23] but intended for wrapping quantum kernels as type-safe callable objects. KernelSignature objects are implicitly constructible from qcor kernel functions (see Fig.
oracle_as_function and its usage with phase_estimation). In other words, users can directly pass a kernel by its name to an argument of type KernelSignature.

Another advanced yet ubiquitous feature of many high-level programming languages is the lambda expression, which enables anonymous functions with the ability to capture variables from the surrounding scope in addition to specified function arguments. Supporting quantum lambda kernels in qcor enables a more concise syntax for a variety of use cases, as shown in Fig. 1. In this example, the oracle kernel is defined in place by using the newly-added qpu_lambda feature and passed to a generic quantum phase estimation kernel which expects an oracle argument of type KernelSignature<qubit>. We want to note that lambda capture is not required in this case but it is a very useful feature to bind additional variables from the local scope to an otherwise fixed functional signature.

Since the SyntaxHandler extension of Clang is designed for free-standing functions, we need a different set of machinery to handle quantum lambda expression, namely macro pre-processing and LLVM Just-In-Time (JIT) engine. Concretely speaking, the qpu_lambda macro turns the quantum lambda body into a source string which will be JIT-compiled, with proper syntax handling, and returns an internal lambda kernel class instance supporting call-like invocation. By-value or by-reference capture variables, if any, can be appended to the functional signature of the underlying rewritten kernel function using their exact names. This allows us to emulate variable capturing in a free-standing, capture-less qcor function. The qcor lambda object keeps a handle to the JIT-compiled function along with copies of any captured variables, and is therefore able to provide the same invocation functionality as one would see with conventional C++ lambdas. As depicted in Fig. 1, qpu_lambda is compatible with KernelSignature argument type similar to global scope __qpu__ kernel functions.

3 PYTHONIC KERNEL PROCESSING IN C++

The first step in creating our Python language extension is to extend the qcor kernel processing infrastructure with support for a Pythonic quantum assembly dialect. Specifically, we will attempt to provide the same functionality inherent to the C++ XASM dialect (simple quantum instructions and C++ control flow, variable assignment, class instance method invocation, etc.), but with a syntax that will ultimately be valid with respect to the Python interpreter. To do this, we implement the TokenCollector interface and override the collect() method, see Fig. 2, to analyze incoming Pythonic quantum assembly tokens (clang:::Token) and provide a re-written source string for use by the Clang SyntaxHandler infrastructure.

```cpp
__qpu__ void phase_estimation(qreg q,
   KernelSignature<qubit> oracle) {
   ...
   // Omitted
}

__qpu__ void oracle_as_function(qubit q) {
   T(q);
}

int main(int argc, char **argv) {
   auto q = qalloc(4);
   // Provide oracle as function
   phase_estimation(q, oracle_as_function);
   // Provide oracle as a lambda
   int capture_int = 5;
   auto oracle =
      qpu_lambda([](qubit q) {
         print(capture_int);
         T(q);
       },
       capture_int);
   phase_estimation(q, oracle);
}
```

Fig. 1. Here we show how one can write quantum kernels parameterized on other quantum kernels via the KernelSignature<...> type. We also leverage this for passing quantum lambda expressions.

Fig. 2. We use the TokenCollector interface and collect tokens by using the collect() method to process Pythonic quantum assembly dialect tokens.

3 PYTHONIC KERNEL PROCESSING IN C++

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Ultimately the goal of this TokenCollector is to map incoming Pythonic quantum code into corresponding C++.

There are a few key challenges in performing this mapping. The first is that Python does not use line terminators like semicolons and tabs or indents are used to indicate new blocks of code instead of braces. Additionally, for and if statements have a different syntax than languages like C and C++. Fortunately, we can work around these issues using the API provided by clang::Token and the clang::SourceManager. Each Token exposes a getLocation() method, which will return information about the token’s source location as a SourceLocation instance. The SourceManager provides methods for querying the token SourceLocation line and column number. With this information, our token analysis is able to know when a new statement has been encountered (line number) and when we enter a new scope or block of code (column number).

We provide a PyXasmTokenCollector implementation of TokenCollector which implements the following mapping strategy: (1) decompose the incoming clang::Tokens into a list of lines or Python statements and associate each line with its corresponding column number, and (2) for each line, we will parse that line to a corresponding parse tree, walk that tree, and map pertinent nodes to C++ equivalents.

For this second part, we leverage the Antlr [24] parser-generator library using the provided C++ runtime. We generate our parser based on the publicly available Python3.g4 grammar specification and implement a custom parse tree visitor that will visit certain nodes and perform the mapping to C++.

Overall, our mapping implementation will handle two types of nodes: (1) quantum instructions and (2) classical instructions. The key Python syntax tree node, which we need to handle, is the atom expression node representing call-like expressions. By inspecting the input tokens at this node, we can distinguish if the function call is a quantum intrinsic instruction, a quantum kernel call, or a classical function call. The first case includes basic quantum gates, such as Hadamard, CNOT gates, etc., which could be identified by matching the name token to the gate registry. The second case is when users make a call to another quantum kernel or their derivatives (controlled or adjoint). There is a special syntax rewrite rule for this case to chain the execution context of this kernel to its sub-kernels, hence

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requiring a custom syntax handling procedure. If no patterns match, then we assume that this is a classical function call to utility helpers provided by the QCOR runtime library and keep the function call intact. Control flow nodes, such as if and for statements, are also converted to their C++ equivalents.

As previously described, we have a stack data structure to keep track of the scope of each code block in order to inject the braces into the rewritten source as appropriate. To rewrite assignment-like statements (e.g., \( a = f(b) \)), we keep track of known variables to inject inline variable declarations (via C++ auto type keyword) when necessary. This is an example of low-level semantic transformation rules that we implemented to bridge Pythonic imperative expressions to a C++ static source. Except for Measure instructions, quantum instructions and kernels don’t have return values, thus do not involve in these assignment statements.

Fig. 4 is an example of the rewritten source code generated by the QCOR syntax handler. The Pythonic body of the bell kernel in Fig. 3 is transformed into a call operator of a qcor QuantumKernel subclass. Specifically, quantum instructions are lowered into concrete quantum runtime functions. Similarly, the Python for loop is converted into a valid C++ equivalent with proper scoping by braces.

Kernel invocation is triggered automatically by the destructor, see [23] for a detailed discussion about the QCOR execution model. Essentially, the PyXASM handler has transformed the Pythonic quantum kernel into a native QCOR QuantumKernel subclass, which could be compiled and linked with the QCOR C++ runtime.

4 QUANTUM JUST-IN-TIME COMPILATION

Having a TokenCollector utility that can turn Python-like source strings into valid C++ code, we now turn our attention to the just-in-time compilation capability of the qcor compiler. For this purpose, we put forward a QJIT class (Quantum Just-in-Time) which loads a quantum kernel source string containing any qcor-supported dialects and maps it to executable binary code in memory, at runtime. The results of successful QJIT compilation are callable function pointers that can be invoked from C++ or Python.

At the high-level, QJIT provides a jit_compile method taking as input a source string. This string captures a quantum kernel in any qcor-supported dialects, such as XASM, OpenQASM, or PyXASM.

```cpp
class bell :
  public qcor::QuantumKernel<class bell, qreg> {
    protected:
      void operator()(qreg q) {
        ...
        quantum::h(q[0]);
        quantum::cnot(q[0], q[1]);
        for (auto i : range(q.size())) {
          quantum::mz(q[i]);
        }
      }
    }
  public:
    bell(qreg q) : QuantumKernel<bell, qreg>(q) {}
    bell(std::shared_ptr<qcor::CompositeInstruction> _parent, qreg q) :
      QuantumKernel<bell, qreg>(_parent, q) {}
    virtual ~bell() {
      ...
      operator()(q);
      ...
    }
  }

public:
  void bell(qreg q) : QuantumKernel<bell, qreg>(q) {
   ...
    bell(std::shared_ptr<qcor::CompositeInstruction> parent, qreg q) {
      class bell __ker__temp__(parent, q);
    }
}

Fig. 4. Syntax handling result of the PyXASM kernel in Fig. 3.
Additionally, we can specify a list of kernel names as dependencies, whose bodies will be pulled in during compilation. This dependency injection mechanism allows us to support nested quantum kernels in the JIT context, whereby kernels are submitted to the QJIT engine individually. Additionally, we allow for extra source code and header include directives to be customized if necessary. The overall execution flow of the `jit_compile` procedure is described in Algorithm 1. When a source string is presented to QJIT, it will first execute the syntax handler to translate that invalid quantum source into valid C++ code, and then compile that rewritten C++ representation to an LLVM IR Module. One key feature of QJIT is its ability to cache the results of both stages for future fast look-up (compile once and reuse the same resultant bitcode). Moreover, the runtime syntax handler results are also cached in memory for future kernel dependency injection. Specifically, as QJIT compiles a kernel, it also saves the rewritten code. Thus, if this kernel is later called within another kernel, the cached source can be injected without any syntax transformation required. Since QJIT works on a kernel-by-kernel basis, this runtime cache eliminates any unnecessary syntax processing when the just-in-time kernels are nested.

Secondly, the compilation result, in terms of the LLVM IR bit-code, is cached permanently on disk. We use the hash digest of the source as the look-up key to the bit-code file. Therefore, future recompiations of the same kernel can be bypassed by loading the IR from files, as shown in the conditional block of Algorithm 1. This caching mechanism is valuable for the Python use case that we are targeting because the LLVM compilation will only occur once, no matter how many times the Python script with embedded kernels is run. The first time a kernel is seen will result in a longer JIT compilation time, but future invocations of that kernel will be fast due to the runtime loading of cached LLVM bit-code files.

## 5 Extending Python via QJIT

Equipped with the syntax handling and just-in-time facilities, the qcor compiler infrastructure can be extended to Python. In particular, we want to translate quantum kernels written in the PyXASM dialect along with a subset of Python language features into binary machine code at runtime. Our goal here is to extend the QCOR single-source programming model to Python programmers and thus allow them to explore QCOR or prototype quantum kernels in a familiar setting (e.g., in IPython notebooks). In particular, users should be able to utilize common Pythonic language constructs like control flow, e.g., Python `if` statements and for loops, utility functions, such as `range` or `print`, and, more importantly, high-level libraries like `numpy` and `openfermion`. Thanks to their linkage to the qcor runtime libraries, the execution of these Pythonic quantum kernels is then seamlessly integrated (just-in-time) with the optimization, placement, and remote job submission pipeline.

Our quantum just-in-time compiler (qjit) in Python operates in three phases: (1) capturing functions intended to describe quantum kernels by means of Python decorators, (2) delegating the compilation of...
the quantum kernel body to the qcor QJIT compiler, and (3) invoking the compiled functions with runtime parameters provided in Python. In the following, we will describe each of the above tasks in detail.

5.1 Python Kernel Decorator - qjit

Since Python is an interpreted language, it is not compatible, out-of-the-box, with the whole kernel source compilation approach of the qcor compiler. It is also worth noting that implementing quantum runtime imperatively via a binding layer is viable but incurs the performance overhead associated with the Python interpreter.

Fortunately, Python provides a decorator utility, which is part of the language, as a means to apply a transformation to a function. In other words, we can decorate a Python function to redirect the execution of that function to an alternative implementation that we provide. Specifically, in the qcor context, we provide a decorator to record the Python kernel function body and pipe it to the QJIT compiler, as described in the previous section, to create a binary function backed by the qcor runtime.

Fig. 5 depicts a decorated quantum kernel whereby qcor provides a qjit decorator implementation activated by the shorthand @ symbol. When the interpreter process this function, it will effectively construct a qjit class instance providing the name and signature of the wrapped function to the constructor. This provides an opportunity for qcor to introspect the function body and analyze the function arguments. The qjit class provides an internal __call__ method for invocation of the JIT-compiled function which the Python kernel is mapped into.

5.1.1 Type Inference. As an dynamically-typed language, Python functions are polymorphic in their inputs, i.e. the number of arguments and their types are flexible. Hence, mapping these functions to qcor kernels, which are strongly-typed C++ functions requires some specific constraints to be enforced upon the decorated function.

First, we require that all function arguments are annotated with type hints. Our Python JIT compiler takes an eager approach, i.e. compiling the kernel at the time of declaration rather than invocation. Therefore, we do not infer the argument types from the specific values provided at the call site. We note that in the vast majority of use cases, qcor users only need to define quantum kernels with fixed argument types. Hence, providing concrete type information enables type-checking, improves kernel declaration readability, prevents any potential type-inference ambiguity, and simplifies our qjit implementation.

Second, the Python-to-C++ type mapping information must be statically provided. In other words, we provide a map from Python types to their C++ equivalents for commonly-used types, including fundamental types (e.g., integer and floating-point numbers), QCOR types (e.g., Operator, qreg, etc.), and containers (list/array) of those types. We use this map to construct the C++ function signature compatible with the qjit kernel, thus runtime arguments provided when invoking the decorated function can be unpacked by the JIT-compiled binary.

We also want to note that qjit kernels support both pass-by-value and pass-by-reference argument types. Since Python does not support passing simple arithmetic types, e.g., integers or floating-point numbers, by reference, we have a custom introspective mechanism to support pass-by-reference for qjit kernel arguments. Using the type annotation data whereby we have defined new reference types that qjit supports, qjit generates the appropriate native (C++) QuantumKernel signature, i.e., deducing the argument type to be a C++ reference type (Type&), see Fig. 4. Having the correct QuantumKernel signature, we turn our attention to the argument reference passing in the Python-C++ interop layer. Ultimately, the
Extending Python for Quantum-Classical Computing via Quantum Just-in-Time Compilation

Pythonic qjit makes copies (pass-by-value) of simple-type arguments when packing runtime variables for invocations. Thus, we need a mechanism to persist these by-reference values across the Python-C++ boundary. Fortunately, qcor quantum kernels, by definition, should always take a qreg as the first argument. Taking advantage of the fact that Python objects are always passed-by-reference, we persist any other by-reference variables to the input qreg at the end of the kernel execution by injecting extra code during qjit decoration handling. At invocation time (qjit’s __call__), we introspect the Python interpreter’s stack frames to determine the outer scope variables that are passed by reference to the qjit kernel. After the JIT kernel execution, we unpack the updated values stored in qreg and assign them to these Python variables accordingly. This passing-by-reference feature is relevant to the FTQC runtime, whereby results of measurement can be accessed in real-time and can be passed around between nested kernels or to the calling code using argument references.

5.1.2 Closure Analysis. The qcor qjit decorator is capable of capturing inputs over the scope of the decorated function and passing them to the C++ JIT kernel. The common use case is numerical constants that users declared outside the scope of the function, i.e. at the global scope of the Python script. By examining the interpreter stack, we record any global variables that are defined and inject those variables into the rewritten source as local definitions. Another common scenario where lexical capture is required is Python module import aliasing. During the processing of the decorated kernel, we resolve any library import alias names to their original name. For instance, if users alias numpy with a very custom name and use the library via this alias in the kernel body, qjit will be able to resolve it back to the original numpy name before the source is passed to the PyXasm syntax handler and ultimately the C++ JIT compiler.

5.1.3 Dependency Analysis. The qcor qjit decorator supports kernel composition allowing users to define quantum kernels in a modular fashion. For example, kernels can call each other so long as there is no circular dependency created. Since we decorate and JIT-compile each kernel separately, the qcor Python library has a mechanism to detect and analyze this dependency information and then provide it to the QJIT’s jit_compile method as explained in the previous section. Fig. 6 (top) is an example of such a scenario whereby there are four kernels, a, b, c and d, that are inter-dependent. The relationship between them can be expressed via a directed acyclic graph (DAG) as shown in Fig. 6 (bottom).

When the qjit constructor is activated and provided with the kernel body, qcor will scan its content to pick up any calls to known kernels which have been presented to the JIT compiler as decorated functions. This scan also covers usage of the controlled or adjoint versions of a kernel which are automatically generated by qcor. For example, kernel d in Fig. 6 makes use of the conjugate of kernel c via the adjoint() method. The relationship between kernels is built up internally as the Python interpreter parses the script and delegates...
kernel functions to qjit. Using a topological sorting algorithm, we can determine the logical ordering of each kernel dependency to provide to the jit_compile function. As noted in Sec. 4, QJIT will pull the transformed source of these dependencies from the cache when constructing the LLVM JIT module.

5.2 Execution Model
All the processing via Python’s decorator utility discussed thus far occurs at the point of kernel definition. The results of this procedure are a decorated Python function (as a Python qjit object) and a binary-compiled function that has been loaded into the memory. Via the binding layer, the qjit object has a handle to the native QJIT instance which kept pointers to those JIT-compiled kernels. When the kernel is invoked, the interpreter will delegate the invocation to the qjit instance’s __call__ method and pass along all the runtime arguments provided at the call site. To bridge the gap between the variadic nature of kernel arguments and the statically-defined binding interface of the native QJIT host, we make use of the heterogeneous map utility of XACC, which models the Python dict type, as the argument container. This heterogeneous container stores argument values indexed by their names, which will later be unpacked in a strongly-type manner using the type information provided previously during the JIT compilation procedure.

Kernel execution occurs entirely at the natively-compiled binary level, i.e., no back-and-forth interaction with the Python interpreter. The underlying execution pipeline includes building up the quantum circuit IR tree, applying optimization/placements passes, and submitting the circuit IR to the XACC Accelerator instance (simulator or cloud-based quantum backends). Quantum runtime configurations, such as shot count, backend name, or optimization parameters, can be specified either as command-line arguments (when invoking the whole script with the Python executable) or via API functions that can be used in the script body. Execution results are persisted to the qreg object which is the required first argument for all qcor kernels.

As described in [23], qcor also supports a tightly-coupled execution model, so-called FTQC, allowing for fast feedback of quantum measurement results. qjit-decorated kernels can also be executed on this FTQC runtime. For instance, kernel arguments can be passed by reference in order to pass real-time measurement-controlled values between kernels or between a kernel and host code (pure Python code). One minor feature that we also want to mention is the ability of the syntax handler to translate Python print function to a C++ equivalent. Thus, users can inject debug printouts into their Python FTQC kernels and observe the console log when the JIT-compiled binary of them is executed.

5.3 Circuit Synthesis Extension
In [23], we have introduced the unitary matrix programming capability (decompose) of qcor (C++) whereby users can specify a circuit block in terms of its unitary matrix representation. Similarly, we also expose this unitary decompose functionality to Python qjit

@qjit
def ccnot(q : qreg):
    ....
    with decompose(q) as ccnot:
        # Create an 8x8 identity matrix
        ccnot = np.eye(8)
        # Modify some entries to create a CCNOT
        ccnot[6,6] = 0.0
        ccnot[7,7] = 0.0
        ccnot[6,7] = 1.0
        ccnot[7,6] = 1.0

        # Other instructions, e.g. Measurement
        ....

Fig. 7. Using the automatic circuit synthesis extension. We overload the standard Python with statement with a special syntax to request circuit synthesis of arbitrary unitary matrices. The with block is translated to a gate sequence at invocation.
as shown in Fig. 7 where we overload the standard Python with statement to handle a special decompose token. The name of the unitary matrix variable, whose body is constructed in the with statement scoped block, is given after the as keyword. We also want to note that the content of the unitary matrix can be constructed in a native Pythonic way, e.g., via math libraries, such as numpy or scipy [28], or quantum libraries, such as cirq [8], OpenFermion [20], etc. Various unitary synthesis techniques are available in qcor, such as kak [15], qfast [29], qsearch [7], qfactor [27], etc. If not specifically given in the decompose call after the qubit register, as the sample in Fig. 7, the default method (qfast) will be used. The with decompose code block is completely equivalent to a sub-circuit, i.e., other quantum instructions can be placed before and after this block when constructing the qjit kernel.

5.4 Compute-Action Extension

As described in 2.1.1, the compute-action-uncompute pattern is commonly used to construct quantum computing algorithms. Through the aforementioned extension to the qcor C++ runtime we are able to enable this feature in Pythonic qjit kernels in a straightforward manner. Similar to the unitary synthesis syntax, we define special with statements to define the scoped blocks of compute (\( U \)) and action (\( V \)). These blocks will be rewritten to the equivalent C++ brace-enclosed compute-action syntax.

Being able to represent this at the programming language level contributes to the improvements of syntax clarity and circuit generation performance. Fig. 8 is an example of using the compute-action-uncompute pattern in a qjit kernel. The compute block (\( U \)) is scoped within a 'with compute' block followed by a 'with action' block describing the action unitary (\( V \)). It is immediately evident that the ability to inject the uncompute sub-circuit (\( U^\dagger \)) automatically shortens the kernel description and makes the programmers' intent clearer.
More importantly, the compute-action annotation allows for optimal generation of the controlled version of the original kernel. In particular, we only need to apply control on the $V$ unitary, thus significantly simplify the circuit. For instance, the quantum circuit of controlled $u_{c1}$ in Fig. 8 is shown in Fig. 9 whereby controlling action is only required for the central $R_z$ gate.

5.5 Pythonic Kernel Callable - KernelSignature

As described in 2.1.2, the QCOR language allows users to pass quantum functions, i.e., kernels or lambdas, as arguments of type KernelSignature capturing the required invocation signature. In Python, we also expose an equivalent syntax as depicted in Fig. 10, whereby a generic Grover’s algorithm kernel takes another kernel describing the quantum oracle operation. Invoking the top-level kernel, in this case, involves providing a subkernel as its argument.

Since qjit-wrapped kernels are pure Python objects, they are not compatible with native JIT-compiled kernel calls. In other words, it is illegal to invoke run_grover with the $cz$ oracle qjit object once run_grover is translated into the JIT function pointer. Technically, what we want to provide as the KernelSignature argument instead is the binary function pointer of $cz$ oracle. Thanks to the KernelSignature type annotation, we can reliably perform this transformation by querying the function handle (pointer) of the callable qjit variable provided at the call site (\_\_call\_ method) and replacing the qjit objects with its native function pointer in the variable pack.

As shown in Fig. 10, to specify a Pythonic KernelSignature type, we provide a variadic list of argument types that the callable kernel expects. This information is necessary for later reconstruction of the underlying templated C++ KernelSignature argument from the JIT-compiled function pointer. We also want to note that automatic adjoint and control modifiers are available to callable arguments similar to a kernel calling other kernels from the global scope. Syntactic differences for kernel modifiers, i.e., static class functions or member functions, at the code-generation layer are distinguished based on the scoping information of the variable, e.g., a global kernel instance vs. a variable declared in the local scope.

![Fig. 10. Passing Python qjit kernels as arguments of type KernelSignature. Specifically, the run_grover kernel implements a generic Grover’s algorithm for arbitrary quantum oracles provided as a callable argument.](image-url)
Table 1. List of notable qjit decorator class utility member functions.

| Method            | Description                                                                                                                                 |
|-------------------|--------------------------------------------------------------------------------------------------------------------------------------------|
| extract_composite | Convert this qjit quantum kernel into an XACC CompositeInstruction. The returned CompositeInstruction is the final IR tree at the gate-by-gate level retrieved from the QCOR runtime after all internal processing such as optimization and placement. This CompositeInstruction is equivalent to the circuit that would be executed on the selected backend if the kernel is invoked. |
| print_kernel      | Print the resolved CompositeInstruction of this qjit kernel to the console.                                                                 |
| openqasm          | Get the OpenQASM equivalent (as a string) of this qjit kernel.                                                                            |
| as_unitary_matrix | Get the unitary matrix representation of this kernel.                                                                                   |
| observe           | Construct and execute observable circuits using this kernel as the base ansatz. The observable operator is given to this method along with other arguments that the kernel expects. This method returns the final expectation value after aggregating all the sub-circuit results. |

5.6 Decorated qjit Utility Methods

Not only does the qjit decorator class wrapper provide a mechanism to delegate the Python `__call__` invocation to the JIT-compiled kernel, but it also provides opportunities to add extra functionality to the Pythonic quantum kernel as member functions of the decorated qjit object. In Table 1, we list a few notable extra utility member functions that we implement for the qjit class. Rather than executing the qjit kernel in a function-call-like manner, users can use these methods to retrieve its internal representation (e.g., as IR tree, unitarity matrix, or OpenQASM string), or compute an observable expectation on the state that the kernel represents.

6 DEMONSTRATION

6.1 Variational Quantum Algorithms

In this example, we use qjit to construct a quantum kernel representing an ansatz for the construction of a qcor ObjectiveFunction. As introduced in [21], ObjectiveFunction is a formal concept in the QCOR specification describing a prototypical $y = F(x)$ functional form. In the VQE context, $F(x)$ can be the energy function which we want to minimize. Therefore, we need to provide the variational state-preparation circuit (ansatz) as well as the Hamiltonian operator to the ObjectiveFunction generator as shown in Fig. 11a. In this example, the kernel is a custom circuit parameterized by a single variable ($t_0$). The deuteron Hamiltonian ($H$) is expressed in terms of builtin Pauli spin operators ($X$, $Y$, and $Z$). With the ObjectiveFunction constructed from the JIT-compiled ansatz and the Hamiltonian, we can use any classical optimizers, e.g., nlopt [13], mlpack [5], scipy [28], etc., to find the ground-state energy via variational minimization. It is worth noting that rather than using the Optimizer and ObjectiveFunction utilities of QCOR to implement the VQE algorithm, one can also use the observe method of the ansatz qjit-decorated object to compute the expectation value (see 5.6) as the cost/objective value to integrate with any optimization protocols.

The results of running the script in Fig. 11a are shown in Fig. 11b, where we plot the energy values at each optimization iteration using different quantum backends, namely an ideal simulator, a noisy simulator, and a quantum device (ibmq_guadalupe, 16 qubits, quantum volume of 32). The qcor runtime is retargetable, meaning that the same quantum kernel can be executed on any hardware backends.
from qcor import *
@qjit
def ansatz(q : qreg, t0: float):
    X(q[0])
    Ry(q[1], t0)
    CNOT(q[1],q[0])

# Define the Hamiltonian
H = -2.1433 * X(0) * X(1) \ 
    - 2.1433 * Y(0) * Y(1) \ 
    + .21829 * Z(0) - 6.125 * Z(1) + 5.907

# Create the ObjectiveFunction
obj = createObjectiveFunction(ansatz, H, 1)
# Create the nlopt optimizer and run
optimizer = createOptimizer('nlopt')
results = optimizer.optimize(obj)

(a) VQE algorithm with a qjit ansatz

Fig. 11. Variational Quantum Eigensolver using the QCOR specification API and Pythonic quantum kernels annotated with the qjit decorator.

from qcor import *
@qjit
def ccnot(q : qreg):
    # create 111
    X(q)
    # decompose ccnot matrix
    with decompose(q) as ccnot:
        ccnot = np.eye(8)
        ccnot[6,6] = 0.0
        ccnot[7,7] = 0.0
        ccnot[6,7] = 1.0
        ccnot[7,6] = 1.0
    Measure(q)
    # Allocate 3 qubits, run, get result
    q = qalloc(3)
    ccnot(q)
    print(q.counts())

(a) Using qcor unitary decompose to synthesize a quantum circuit for a CCNOT gate.

Fig. 12. Variational Quantum Eigensolver using the QCOR specification API and Pythonic quantum kernels annotated
Hence, users just need to use the -qpu flag to select the QPU backend that they want to run the quantum experiments on. With an ideal simulator, the observable converges to the expected ground-state energy of deuteron. There is a slight deviation from the theoretical value due to gate noises and readout errors when executing the VQE loop on real hardware. Using a noisy simulator, taking into account the device model, we can reproduce the hardware results with very high fidelity, indicating that the hardware imperfections are well-characterized by the calibration procedure.

6.2 Circuit Synthesis

In this example, we want to demonstrate the circuit synthesis functionality of qcor whereby a sub-circuit is described by its unitary matrix as shown in Fig. 12b (top). Here, the unitary matrix represents a doubly-controlled NOT gate (CCNOT). We add X gates before the CCNOT block to examine the truth table of the decomposed circuit. For instance, when all qubits are in |1⟩ state, we expect the result to be |011⟩, i.e., the target qubit (MSB) is flipped from |1⟩ to |0⟩. Fig. 12b (bottom) shows the bit-string distribution from executing the circuit (8192 shots) on the IBMQ Yorktown device for the initial states of |111⟩ and |011⟩. We expect transitions from |011⟩ to |111⟩ and vice-versa, which are evident in the distributions in Fig. 12b (bottom). We want to note that this decomposition is using the QFAST [29] algorithm and is mainly for demonstration purposes since there exists better decompositions specifically for the CCNOT gate. The QFAST-decomposed circuit contains more than 40 CNOT gates\(^1\) which contribute to noisy distribution results.

\(^1\)Avg. CNOT Error: 2.14e-2

```python
from qcor import *
@qjit
def ansatz(q : qreg, x : List[float]):
    X(q[0])
    with decompose(q, kak) as u:
        from scipy.sparse.linalg import expm
        from openfermion.ops import QubitOperator
        from openfermion.transforms import get_sparse_operator
        qop = QubitOperator('X0 Y1') - QubitOperator('Y0 X1')
        qubit_sparse = get_sparse_operator(qop)
        u = expm(0.5j * x[0] * qubit_sparse).todense()

# Define the Hamiltonain
from openfermion.ops import FermionOperator as FOp
H = FOp('', 0.0002899) + FOp('0^ 0', -.43658) + FOp('1 0^', 4.2866)
    + FOp('1^ 0', -4.2866) + FOp('1^ 1', 12.25)

# Create the VQE ObjectiveFunction
vqe_obj = createObjectiveFunction(ansatz, H, 1)
# Create an optimizer (gradient free)
optimizer = createOptimizer('nlopt')
# Find the ground state via optimization
results = optimizer.optimize(vqe_obj)
```

Fig. 13. VQE algorithm where the ansatz circuit is described in terms of a matrix constructed using Scipy and OpenFermion. The Hamiltonian observable is also expressed as FermionOperator.
6.3 Third-party Integration

Through this novel Python language extension, we anticipate that qcor users will be able to incorporate a wide range of libraries into their quantum programming workflows. For instance, Fig. 13 demonstrates the ability to integrate Open-Fermion [20] and Scipy [28] Python packages in a qjit quantum kernel definition.

This example essentially runs the same VQE procedure as the one depicted in Fig. 11a. However, rather than defining the Hamiltonian in terms of qcor Pauli operators (e.g., X, Y, and Z), we use the FermionOperator representation provided in the popular OpenFermion Python package. Internally, qcor has compatibility adapters to convert these library-specific objects into qcor representations.

6.4 Circuit Composition Performance

One of the key design aspects of qcor is its system-level orientation intended for large-scale deployment. Hence, the implementation is entirely based on C++ for optimal performance. In [23], we have demonstrated significant speed-up in terms of quantum circuit composition time between quantum kernels written in C++ and Python.

Since the qjit extension that we presented here is based on JIT compilation into binary code, we expect that the runtime performance of these qjit kernels is on par with their native C++ counterparts. It is worth reiterating that with qjit the whole kernel is wrapped as a binary function handle as described in Sec. 5, hence skipping all the expensive interactions with the Python interpreter during kernel execution.

Table 2. Trotter circuit composition performance (not including PySCF time). Number of Trotter steps = 1. Hamiltonian from PySCF using sto3g basis. We skip the Qiskit run for C2H4 due to time limit.

| Molecule | Qubits | Terms | Instructions | qjit runtime [sec] | Qiskit runtime [sec] |
|----------|--------|-------|--------------|--------------------|---------------------|
| H2       | 4      | 14    | 82           | 0.00465            | 0.1569              |
| H2O      | 14     | 1085  | 17963        | 0.2441             | 22.9048             |
| N2       | 20     | 2950  | 62618        | 0.7128             | 82.6061             |
| C2H4     | 28     | 57092 | 1503664      | 16.84              | –                   |

To evaluate the circuit composition performance of the qjit kernel, we time the trotter_circ kernel runtime, as defined in Fig. 14, against a set of molecular Hamiltonian operators, as shown in Table 2. In this benchmark, we use a fixed number of Trotter steps (one step) and feed the kernel with the Pauli-sum representation\(^2\) of each molecule’s Hamiltonian (generated by PySCF [26]).

The timing data in Table 2 only include the duration of the circuit construction, i.e., from the time the kernel function is invoked to the point when the flattened instruction list is generated. This includes looping over individual terms, generating and appending the exp_i_theta sub-circuits. On average, our JIT-compiled kernel function is 30x-100x faster in constructing the flattened gate IR than a pure Python equivalent. The main contribution to the performance improvement is that, for qjit kernels, all PyXASM constructs, such as for loops, exp_i_theta instructions, are compiled to native C++ binary objects resulting in a highly optimal and efficient execution. This provides a high-performance and scalable

\(^2\)via Jordan-Wigner transformation
quantum programming environment, not only for near-term use cases but also for future large-scale deployments.

### 6.5 FTQC Runtime Execution

In [23], we introduced a fully dynamic quantum runtime for qcor, named FTQC, capable of handling flexible control flow based on real-time measurement results. This runtime is relevant to quantum error correction whereby syndrome measurement results are used to detect and correct quantum errors. Fig. 15 illustrates the FTQC runtime utility in simulating quantum error correction code. In this case, it is a simple three-qubit repetition code toy model which could detect single bit-flip (X) errors by comparing the parities between qubit pairs. The code snippet in Fig. 15 is a qjit kernel subroutine that projects the parity of neighboring qubits (q[0]-q[1] and q[1]-q[2]) into an ancilla qubit. Since the measurement result of this ancilla qubit is immediately available in the FTQC runtime, users can perform arithmetic operations based on bit results as well as conditional gate instructions. Using a simple mapping from parity syndrome to error location, we can then correct a bit-flip error if it has occurred. Despite its simplicity, this example demonstrates the versatility of the qcor programming framework. With the introduction of the OpenQASM version 3, we anticipate that this dynamic quantum programming model will soon become available from hardware providers, and through this JIT extension, Python users will be able to take full advantage of the FTQC runtime to develop and test algorithms on tightly-coupled CPU-QPU machine models.

![Code snippet](image-url)

**Fig. 15.** Apply a quantum-error-correction round on a logical qubit encoded in the three-qubit bit-flip code using FTQC runtime. The console logging via `print()` and syndrome calculation reflects the real-time feedback of measurement results available in the FTQC runtime.

### 6.6 Integration with HPC Simulators

The qcor runtime, based on the XACC framework, incorporates a couple of HPC quantum circuit simulators capable of distributing the compute workload across multiple nodes via the Message Passing Interface (MPI). For instance, XACC has a tensor network-based simulator, named TNQVM [22], capable of running on leadership-class supercomputers, such as the Summit supercomputer at Oak Ridge National Laboratory. In this demonstration, we seek to demonstrate the usage of such high-performance simulators to simulate large-scale quantum circuits expressed as qjit kernels.

**Fig. 16a is a code snippet whereby we simulate the seminal random circuit sampling circuit that Google ran on their Sycamore chip (53 qubits) [3]. In this example, we use the `observe` utility of qjit, see Table 1, to compute the expectation of an arbitrary**

200 petaFLOPS, the second fastest supercomputer in the world (as of April 2021)
from qcor import *
@qjit
def rcs_circuit(q : qreg):
...
Rz(q[0], -0.78539816339)
...
Rz(q[52], -1.2305673521313445)
...
fSim(q[47], q[51],
1.490808748931237, 0.4862437201319)
fSim(q[50], q[52],
1.616256997269376, 0.5014289362839901)
...

# Allocate 53 qubits
q = qalloc(53)
# Compute the expectation value
obs = rcs_circuit.observe(ham, q)
------------- Run with -------------
$ mpiexec -n <n_procs> \
python3 sycamore.py \
-qpu tnqvm[qcor_qpu_config:<config_file>]

(a) Simulating qjit kernel on HPC simulator (TNQVM). The quantum kernel is a random circuit sampling (RCS) adapting from the Sycamore quantum supremacy experiment involving 53 qubits.

operator. For demonstration purposes, we compute the all-Z ($Z_0 Z_1 ... Z_{52}$) expectation value. This Python script can be executed in an MPI-distributed environment (e.g. via mpiexec) using packages such as MPI for Python (mpi4py) [6] as shown in the running command in Fig. 16a. Another feature that we want to highlight in this example is the ability to pass detailed accelerator configurations in a file to the backend accelerator via the qcor_qpu_config key. This functionality is often required by complex Accelerator implementations, which have customized performance switches, e.g., memory buffer size, task distribution strategies, etc.

A sample performance scaling data is shown in Fig. 16b, where we vary the number of MPI processes to assess the task distribution. We also want to note that this demonstration only uses CPU’s hence not utilizing the full capability of the TNQVM simulator, which could perform tensor processing on GPU’s thanks to its integration with the ExaTN library [1]. As we can see from Fig. 16b, there is a significant performance boost in terms of Flop rate of the ExaTN numerical backend when going from one to two MPI processes, which matches our expectation for this two-socket workstation. The performance saturates when going to higher MPI ranks due to machine configuration. We also want to note that the total runtime includes not only the tensor contraction task, whose Flop count we track, but also other workloads, such as tensor network construction and contraction sequence optimization. For example, the improvement in total runtime in the rank-4 case is mostly due to faster contraction optimization and better contraction path.

4Compute node: 2x AMD EPYC 7302 16-core Processor (3.0 GHz)
Manuscript submitted to ACM
7 CONCLUSION

We have presented a language extension to Python for heterogeneous quantum-classical computing that utilizes quantum kernel just-in-time compilation at the C++ level to ensure a performant execution model. Our work builds upon the qcor C++ infrastructure to enable a single-source programming model for quantum computing that is quantum coprocessor retargetable. Our work seeks to provide a future-proof platform for rapid prototyping and experimentation of quantum scientific computing applications under both loosely and tightly coupled CPU-QPU machine models. We anticipate that this core Pythonic infrastructure can serve as a foundation for rapid experimentation via scripting, application libraries, and benchmarking of quantum-classical use-cases in a hardware-agnostic manner.

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