Quantum Computer Programming, Compilation, and Execution with XACC

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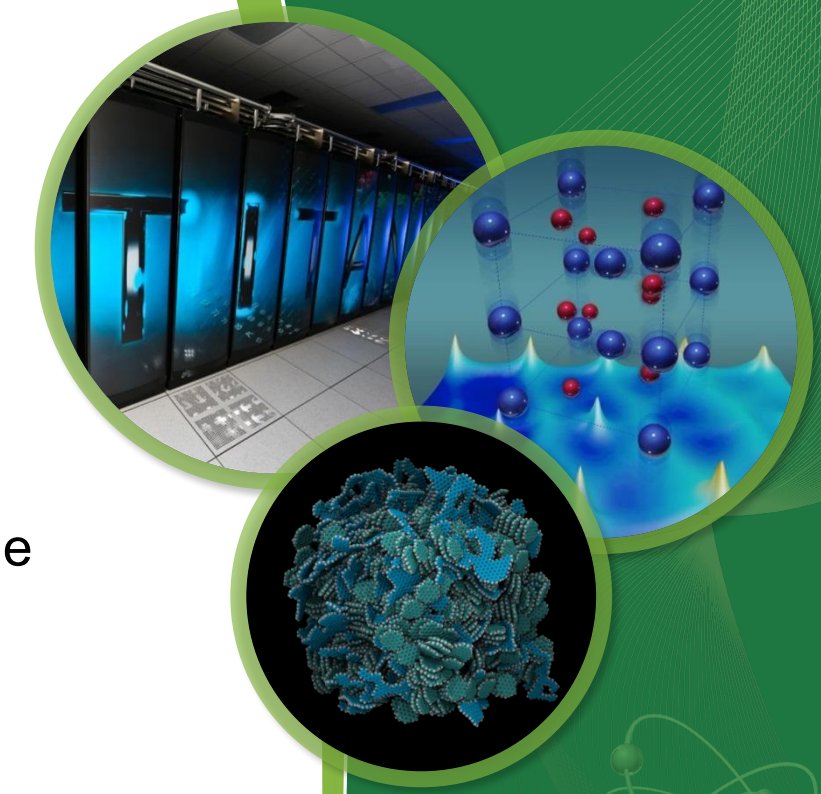

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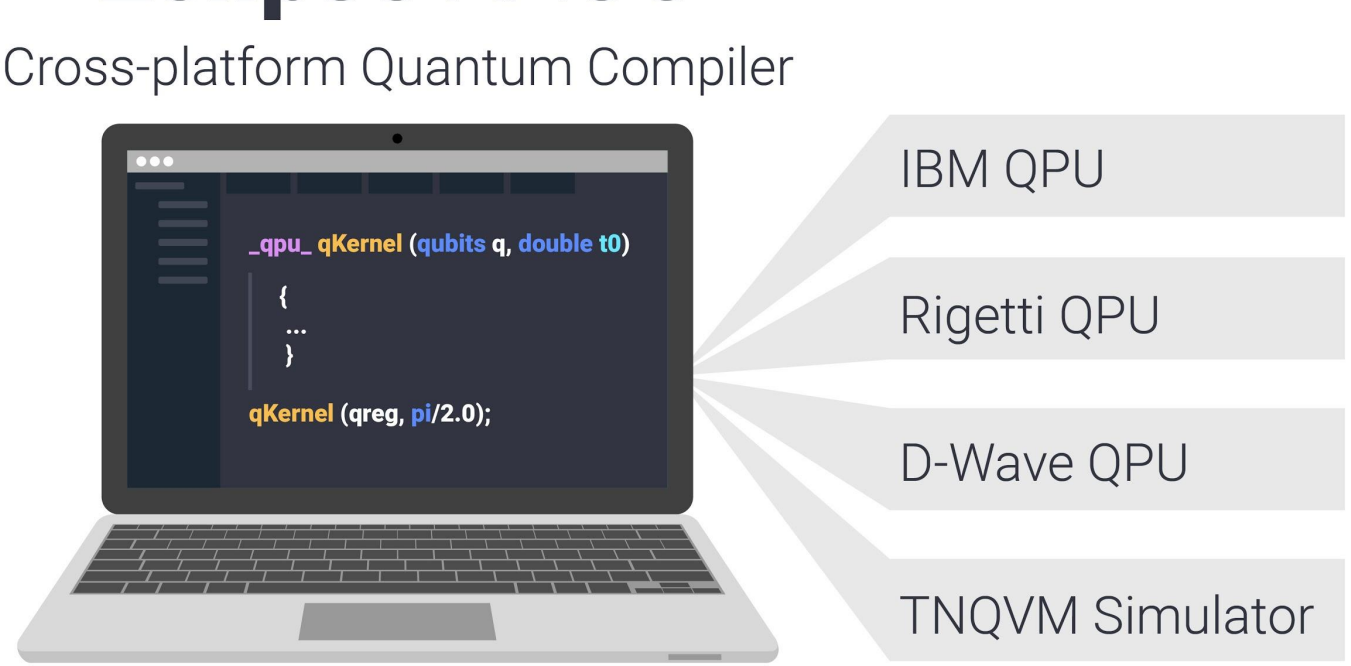
26 September 2018

Outline

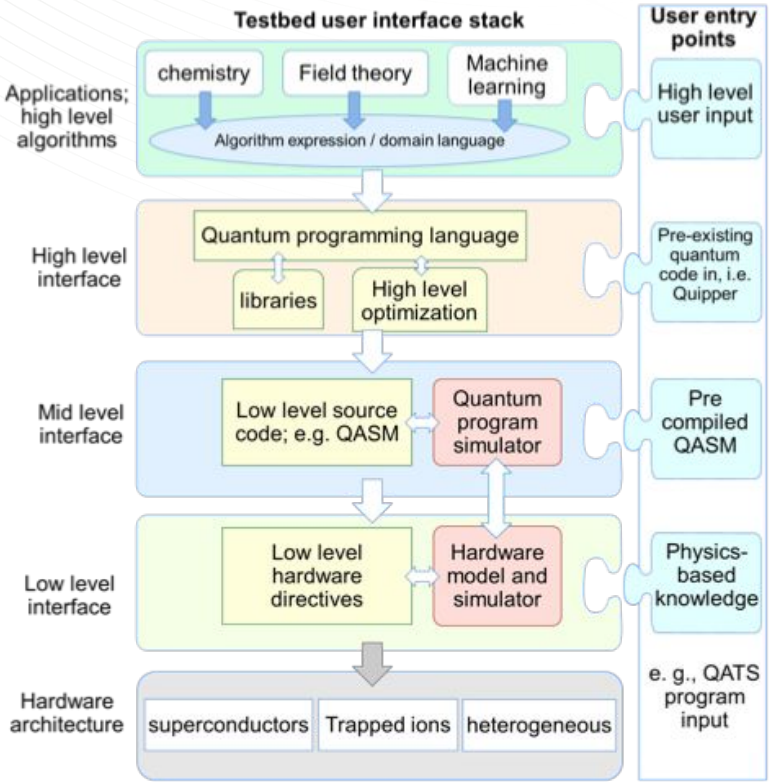
- Motivation, ORNL Requirements
- XACC
  - Birds-eye view and software stack
- Architecture
  - Platform and Memory model
  - Programming model
- Python JIT



Quantum Software Efforts at ORNL

- What is driving ORNL quantum programming efforts?

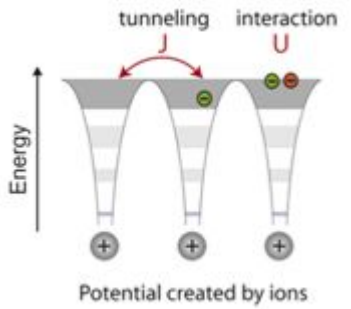
DOE Testbed Project - Materials and Interfaces for Quantum Acceleration of Science Applications (MIQASA)

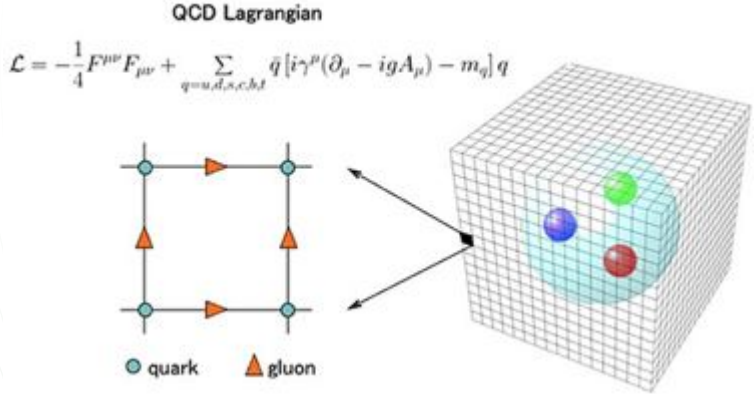


ORNL Programming Requirements

- Anticipation of ORNL Post-Exascale Computing
  - treat QPUs as accelerators
  - leverage wealth of classical co-processor R&D
- MIQASA benchmarking across QPU hardware types
  - enable hardware-independent programming
- HDAQDS execution across QPU types and high-level program expression
  - extensibility in compilation techniques

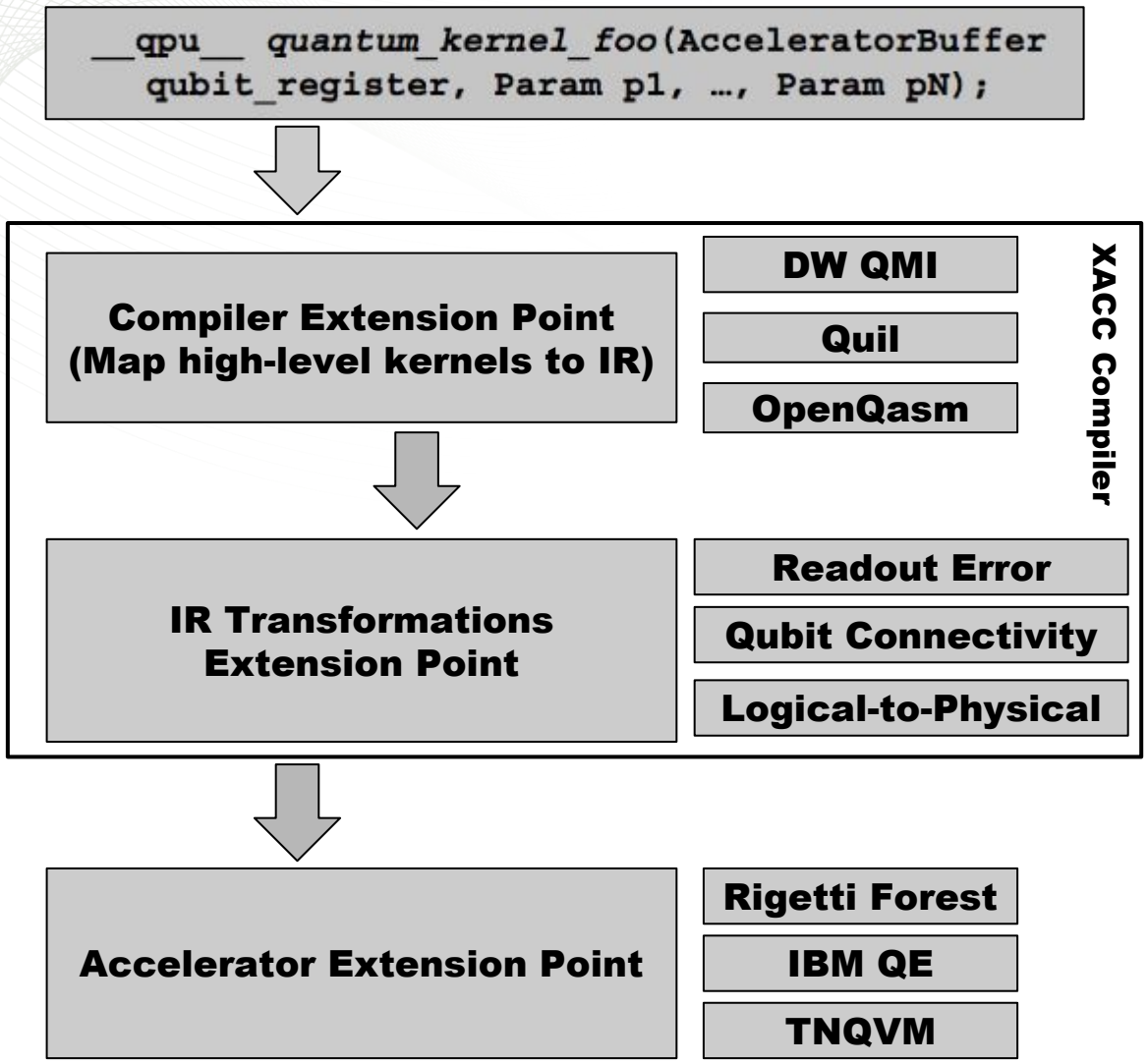
DOE QAT - Heterogeneous Digital-Analog Quantum Dynamics Simulation (HDAQDS)





XACC - Compiler Framework for Quantum Computing

Users define Quantum Kernels (Kernel in the GPU sense, a C-like Function)



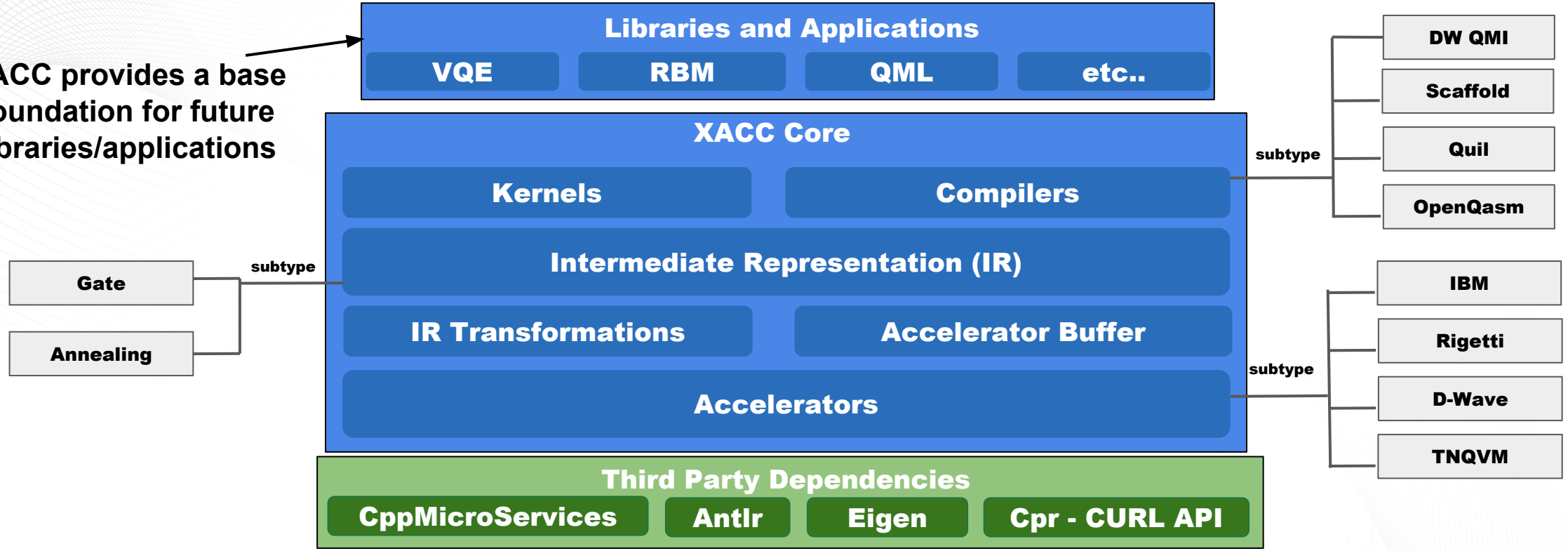
- Open-source at https://github.com/eclipse/xacc
- Familiar API and model
  - OpenCL-like, LLVM-like, hardware and language independent
- Key Abstractions
  - Kernels and Compilers (Frontend)
  - Intermediate Representation (Middle-end)
  - Accelerators (Backend)
- OSGI C++ *modular, service-oriented architecture*
  - Framework Extension Points

```
// Get reference to the QPU, and allocate a buffer of qubits
auto qpu = xacc::getAccelerator("ibm");
auto buffer = qpu->createBuffer("qreg", 2);

// Create and compile the Program from the kernel
// source code. Get executable Kernel source code
auto kernelSourceCode = "__qpu__ foo(double theta) {....}";
xacc::Program program(qpu, kernelSourceCode);
program.build();
auto kernel = program.getKernel<double>("foo");

// Execute over theta range
for (auto theta : thetas) kernel(buffer, theta);
```

XACC Software Stack

Key architectural design: service-oriented, modular, extensible

XACC provides a base foundation for future libraries/applications



- **CppMicroServices**
  - https://github.com/CppMicroservices/CppMicroServices
  - Native C++ OSGI implementation
  - Framework, Bundle, BundleContext abstractions
  - XACC plugins are exposed as Framework Bundles provided at runtime as shared libraries
  - CppMicroServices abstracts away dlload,dlopen,dlsym commands

- **Antlr**
  - Automated Parser Generation for user-defined languages
  - Define EBNF Grammar, generate Parser code
  - Our compilers use Antlr Parsers to generate quantum code AST, then we map AST to XACC IR
- **Cpr**
  - Curl for People :), spiritual port of Python Requests

XACC Architecture

Platform, Memory, and Programming Model

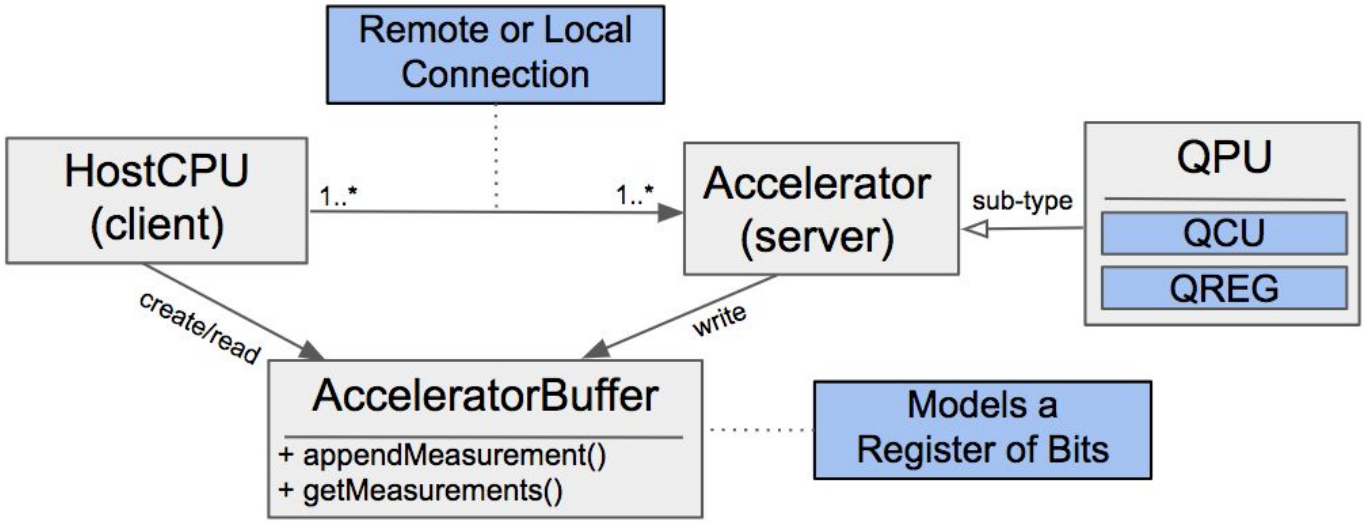
What makes this API possible?

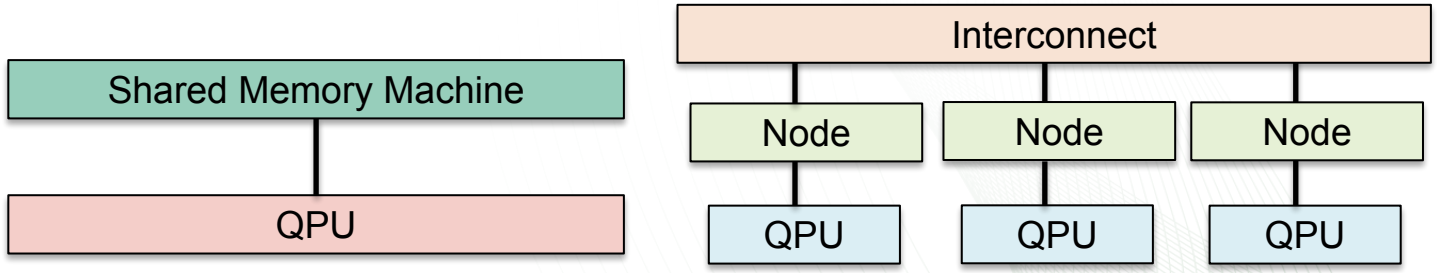
```python
# Get reference to the QPU, allocate a buffer of qubits
qpu = xacc.getAccelerator('ibm')
buffer = qpu.createBuffer('q',2)

# Create and compile the Program from the kernel
# source code. Get executable kernel
kernelSourceCode = '__qpu__ foo(double theta) {...}'
program = xacc.Program(qpu, kernelSourceCode)
program.build()
kernel = program.getKernel('foo')

# Execute over theta range
[kernel.execute(buffer, [theta]) for theta in thetas]
```

```cpp
// Get reference to the QPU, and allocate a buffer of qubits
auto qpu = xacc::getAccelerator("ibm");
auto buffer = qpu->createBuffer("qreg", 2);

// Create and compile the Program from the kernel
// source code. Get executable Kernel source code
auto kernelSourceCode = "__qpu__ foo(double theta) {....}";
xacc::Program program(qpu, kernelSourceCode);
program.build();
auto kernel = program.getKernel<double>("foo");

// Execute over theta range
for (auto theta : thetas) kernel(buffer, theta);
```

XACC Platform and Memory Model

- Platform model, system context
  - 3 primary actors, host CPU, Accelerator, and AcceleratorBuffer
  - client-server model
  - Subtypes of the Accelerator system
- Enables serial and parallel execution contexts
- Enables a number of co-processor integration strategies
  - loose and tight coupling, remote or localhost
- Measurement results shared through AcceleratorBuffer





Programming Model - Kernels

- XACC Kernel definitions are GPU-like (OpenCL, CUDA)
  - familiar mechanism for programming accelerator
- Kernels can be parameterized
  - **`InstructionParameter`** variant data structure (**`float,int,double,string,complex`**)
- Annotated with **`__qpu__`** function attribute for future static, ahead-of-time compiler based on Clang

`__qpu__ quantum_kernel_foo(AcceleratorBuffer qubit_register, Param p1, …, Param pN);`	
XACC Kernel Requirement	**Description**
Annotation	All kernels must be annotated with the __qpu__ function attribute to enable static, ahead-of-time compilation
Kernel Name	All kernels must be given a unique name
Accelerator Buffer Argument	All kernels must take as a first function argument the Accelerator Buffer this kernel acts on.
Runtime Parameters	All kernels can take any number of runtime arguments.

Example XACC Kernels

```
__qpu__ teleport (qbit& qreg) {
    X(qreg[0]);
    H(qreg[1]);
    CNOT(qreg[1],qreg[2]);
    CNOT(qreg[0],qreg[1]);
    H(qreg[0]);
    cbit c1 = MeasZ(qreg[0]);
    cbit c2 = MeasZ(qreg[1]);
    if(c1 == 1) Z(qreg[2]);
    if(c2 == 1) X(qreg[2]);
}
```

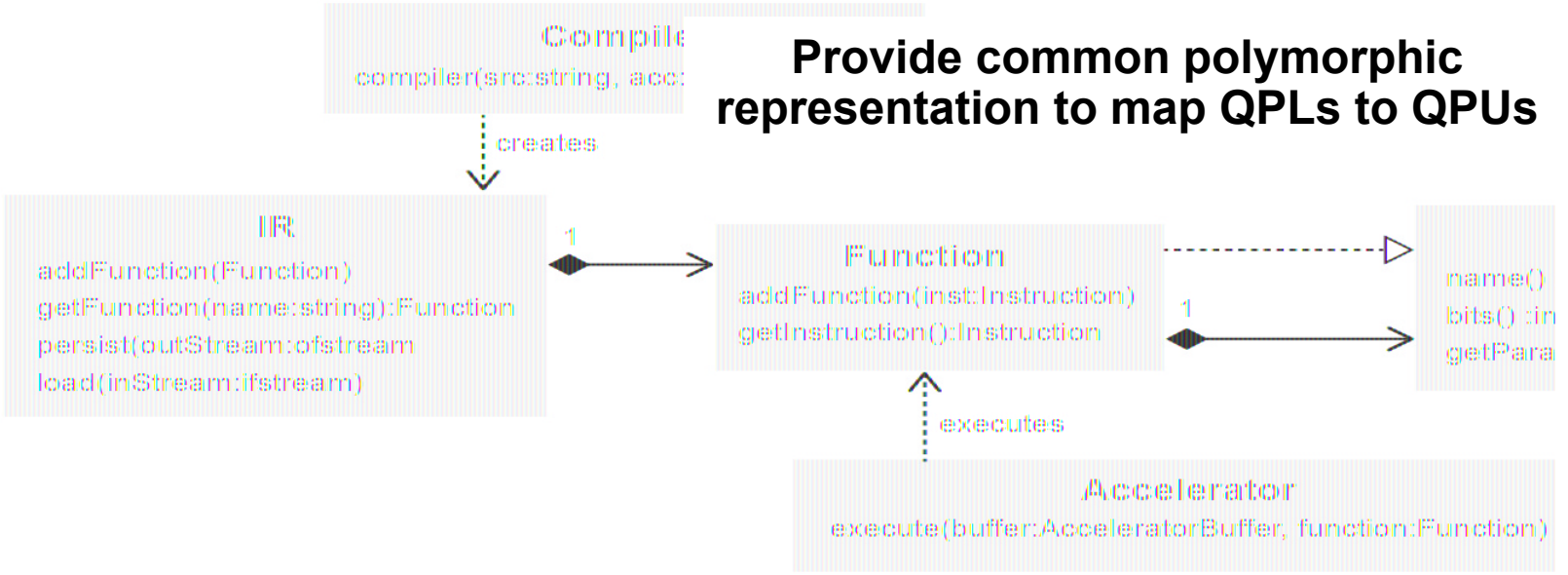
```
__qpu__ variable(AcceleratorBuffer ab, double ta,
                 double tp, double tq,
                 double h, double J) {
    anneal ta tp tq;
    0 0 h;
    1 1 h;
    0 1 J;
}
```

```
__qpu__ ansatz(AcceleratorBuffer b, double t0) {
RX(3.1415926) 0
RY(1.57079) 1
RX(7.85397) 0
CNOT 1 0
RZ(t0) 0
CNOT 1 0
RY(7.8539752) 1
RX(1.57079) 0
}
__qpu__ term0(AcceleratorBuffer b, double t0) {
ansatz(b, t0)
MEASURE 0 [0]
}
__qpu__ term1(AcceleratorBuffer b, double t0) {
ansatz(b, t0)
MEASURE 1 [0]
}
```

```
__qpu__ term2(AcceleratorBuffer b, double t0) {
ansatz(b, t0)
MEASURE 0 [0]
MEASURE 1 [1]
}
__qpu__ term3(AcceleratorBuffer b, double t0) {
ansatz(b, t0)
H 0
H 1
MEASURE 0 [0]
MEASURE 1 [1]
}
__qpu__ term4(AcceleratorBuffer b, double t0) {
ansatz(b, t0)
RX(1.57079) 0
RX(1.57079) 1
MEASURE 0 [0]
MEASURE 1 [1]
}
```

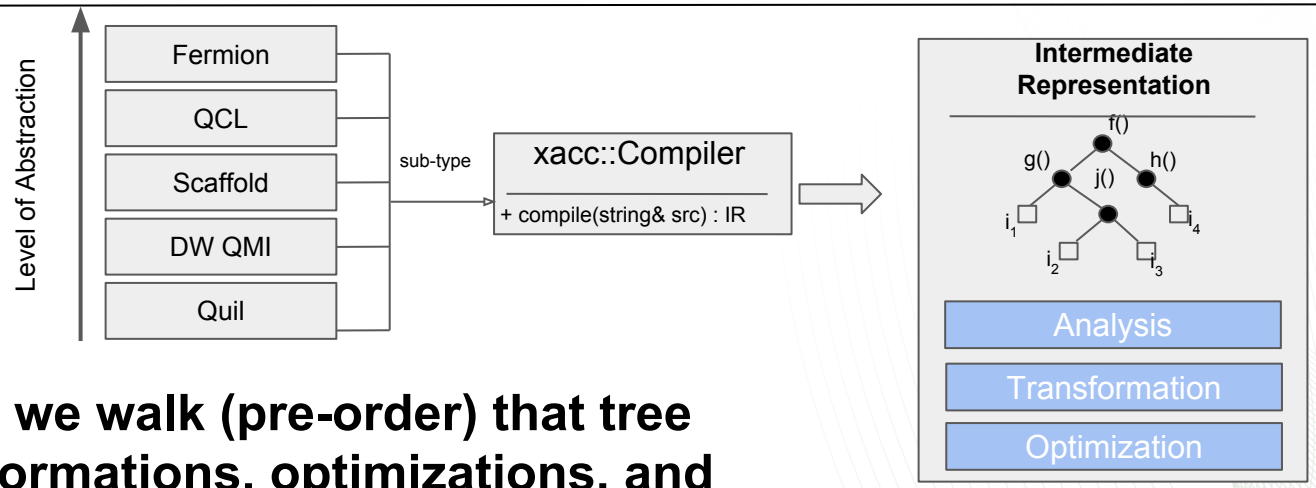
XACC Intermediate Representation

- **Instructions**
  - operate on qubits, unique names, parameterized
- **Functions**
  - Are Instructions but also contain further Instructions - Composite Pattern
  - Compiled representation of Kernel functions
- **IR**
  - Container of Functions, forest of trees
  - IR Transformations and IR Preprocessors



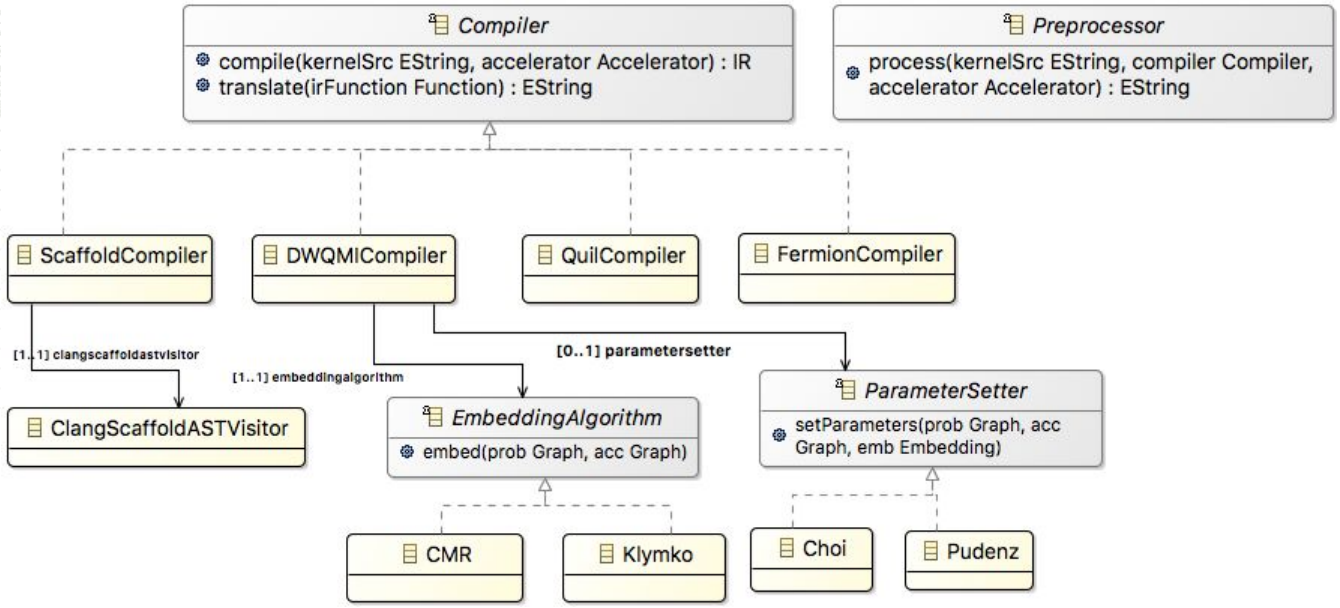
Provide common polymorphic representation to map QPLs to QPUs

```
__qpu__ j(AcceleratorBuffer b) { i2 1; i3 0;}
__qpu__ g(AcceleratorBuffer b) { i1 0; j();}
__qpu__ h(AcceleratorBuffer b) { i4 2;}
__qpu__ f(AcceleratorBuffer b) { g(); h();}
```



XACC IR models an *n-ary tree*, and we walk (pre-order) that tree to perform program analysis, transformations, optimizations, and executions

Programming Model - Compilers and Transpilers

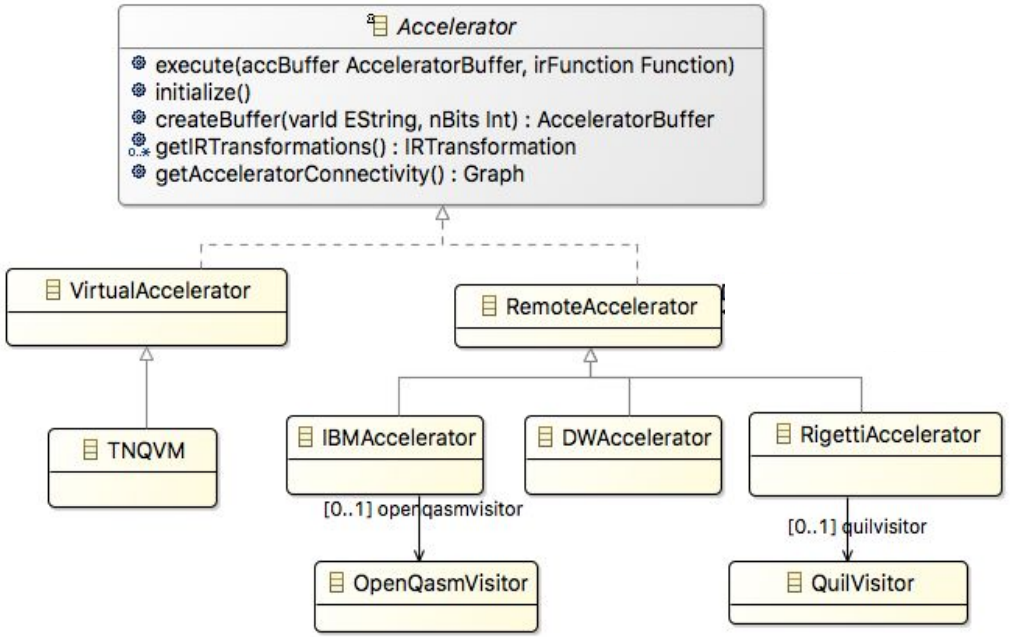


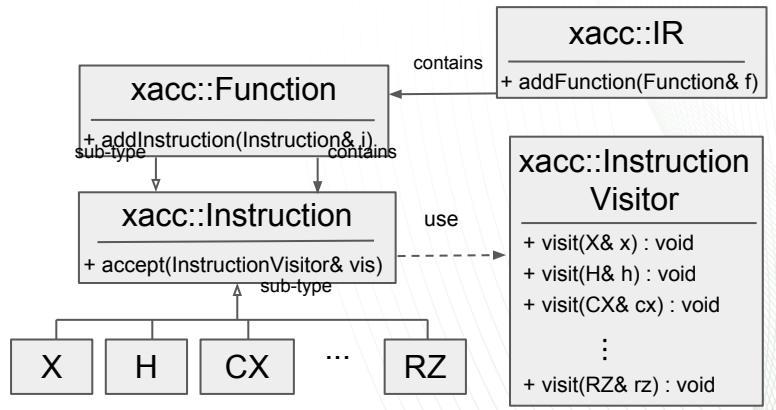
- **D-Wave Compiler** delegates to Antlr for source code parsing
- Provides extension point for minor graph embedding and parameter setting
- Enables **`anneal`** instruction to specify anneal schedule with pause,quench

- Compilers take source code and Accelerator, produce XACC IR
  - Hardware-specific information available at compile time
- Compilers provide source-to-source translation capabilities
  - transpile one hardware instruction set to another
- Extensible Preprocessor mechanism
  - Macro-like functionality

Programming Model - Accelerators

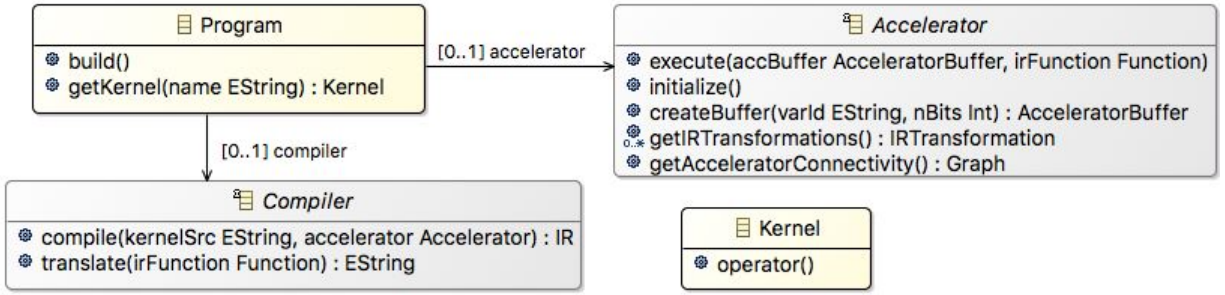
- Accelerators execute XACC IR
- Can be simulators, physical QPUs, remote or local
- Provides **`initialize()`** for costly startup
- Provide hardware-dependent IR Transformations
- Remote Accelerators delegate to remote execution server with CPR CURL API
  - If QPU has REST API, we can target it
- Visitors walk IR, produce native code
  - or apply gates in case of simulation (as done with TNQVM)



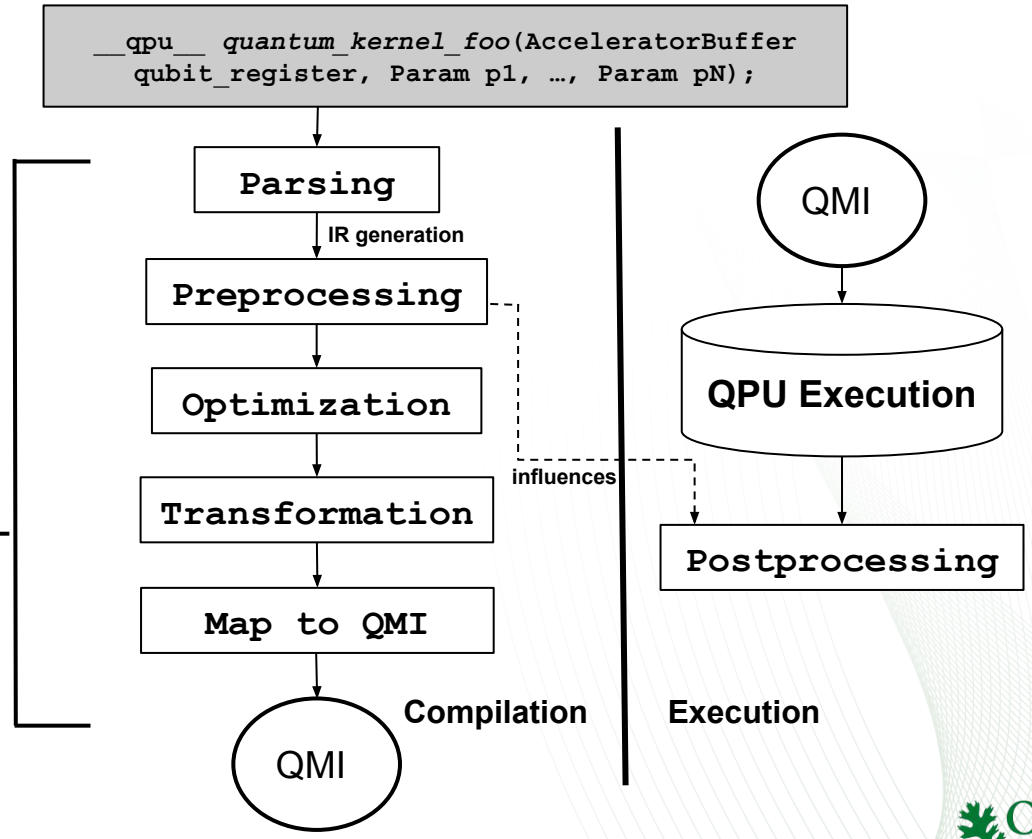


Programming Model - Program

- Programs orchestrate the XACC compilation workflow
  - Execute correct Compiler for the given kernel language
  - Execute IR Preprocessors, Transformations, Optimizations
  - Map to hardware-native QMI
  - Store data post-processors
- Provide an executable lambda (potentially parameterized)




```
// Get reference to the QPU, and allocate a buffer of qubits
auto qpu = xacc::getAccelerator("ibm");
auto buffer = qpu->createBuffer("qreg", 2);

// Create and compile the Program from the kernel
// source code. Get executable Kernel source code
auto kernelSourceCode = "__qpu__ foo(double theta) {....}";
xacc::Program program(qpu, kernelSourceCode);
program.build();
auto kernel = program.getKernel<double>("foo");

// Execute over theta range
for (auto theta : thetas) kernel(buffer, theta);
```



XACC Extensions

XACC Extension Points
Compiler
Preprocessor
Accelerator
Instruction
EmbeddingAlgorithm
ParameterSetter
IRTransformation
IRPreprocessor
AcceleratorBufferPostprocessor
IRGenerator

Extension	Provides
xacc-rigetti	QuilCompiler (leverages ANTLR), RigettiAccelerator
xacc-ibm	OpenQasmCompiler (leverages ANTLR), IBMAccelerator
xacc-dwave	DWQMICompiler (leverages ANTLR and Embeding Algorithm extension point), DWAccelerator
xacc-projectq	ProjectQCompiler (low-level ProjectQ-Qasm transpiler)
xacc-vqe	VQETask, VQEMinimizeBackend, VQEProgram, FermionCompiler, JW and BK IRTransformations, UCCSD IRGenerator
xacc-vqe-fcidump	FCIDumpPreprocessor (map FCIDump format to FermionCompiler)
xacc-vqe-bayesopt	VQEMinimizeBackend implementing bayesian optimization
xacc-cmr	CMR Embedding Algorithm delegating to D-Wave MinorMiner
tnqvm	TNQVM Accelerator (Tensor Network Quantum Virtual Machine), TNQVM Visitor Backend
xacc-atos	ATOSVisitor (mapping IR to ATOS Circuit), ATOSAccelerator

XACC Architecture

What's wrong with the API below?

```python
# Get reference to the QPU, allocate a buffer of qubits
qpu = xacc.getAccelerator('ibm')
buffer = qpu.createBuffer('q',2)

# Create and compile the Program from the kernel
# source code. Get executable kernel
kernelSourceCode = '__qpu__ foo(double theta) {...}'
program = xacc.Program(qpu, kernelSourceCode)
program.build()
kernel = program.getKernel('foo')

# Execute over theta range
[kernel.execute(buffer, [theta]) for theta in thetas]
```

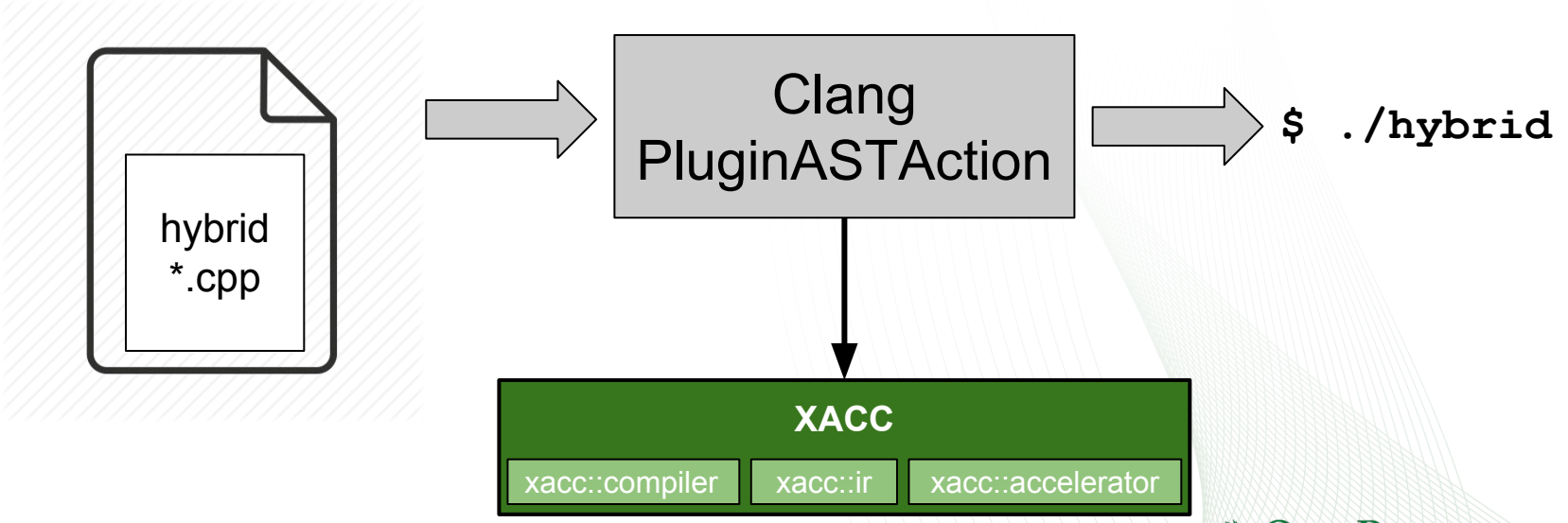
```cpp
// Get reference to the QPU, and allocate a buffer of qubits
auto qpu = xacc::getAccelerator("ibm");
auto buffer = qpu->createBuffer("qreg", 2);

// Create and compile the Program from the kernel
// source code. Get executable Kernel source code
auto kernelSourceCode = "__qpu__ foo(double theta) {...}";
xacc::Program program(qpu, kernelSourceCode);
program.build();
auto kernel = program.getKernel<double>("foo");

// Execute over theta range
for (auto theta : thetas) kernel(buffer, theta);
```

Primarily, kernels provided as strings and too much boilerplate code

Hybrid Quantum-Classical C++ Compiler

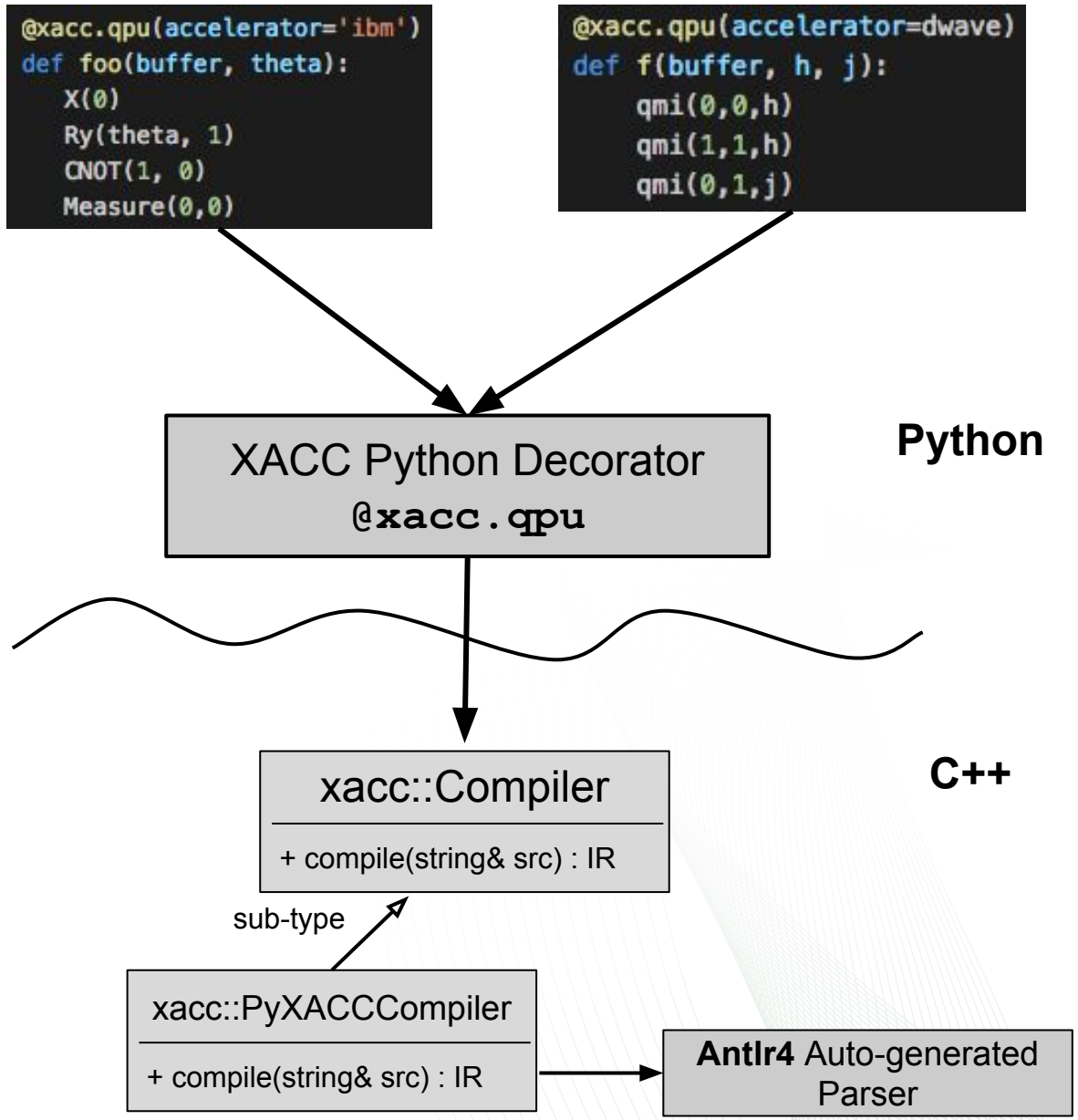
- Run **`xacc`** just like you would **`g++/clang++`**
- Make use of kernel **`__qpu__`** function attribute
- Leverage Clang Plugins or LibTooling
  - Walk clang AST searching for XACC kernels
  - Refactor kernel code to leverage low-level API
- This is something we are currently working on, not available yet.

```
$ cat hybrid_code.cpp
__qpu__ f(AcceleratorBuffer b, double t) {...}
int main() {
    ...
    f(qubits, xacc::pi/2.);
    ...
}
$ xacc hybrid_code.cpp -a ibm -o hybrid
```



XACC Python JIT Compiler

- Goals
  - single-source, so kernel strings
  - unified programming model for available QPUs
  - Single gate+annealing model language
  - IRGenerator instructions
- Requirements
  - language must be Pythonic (to pass interpreter)
  - Users must annotate python functions to indicate intention for QPU execution
  - typical xacc kernel requirements (buffer is first argument)
- How's it done?
  - Python Inspect Module (get source string at runtime)
  - Decorator compiles with XACC PyXACCCompiler, runs usual XACC execution API



XACC Python JIT Compiler and the IRGenerator

- Goals
  - Provide a mechanism for programming complex circuits / QUBOs parameterized by high-level user input
- How's it done?
  - PyXACCCompiler interprets custom **`xacc()`** instruction
    - first argument is the name of the IRGenerator
    - following arguments are the list of user input

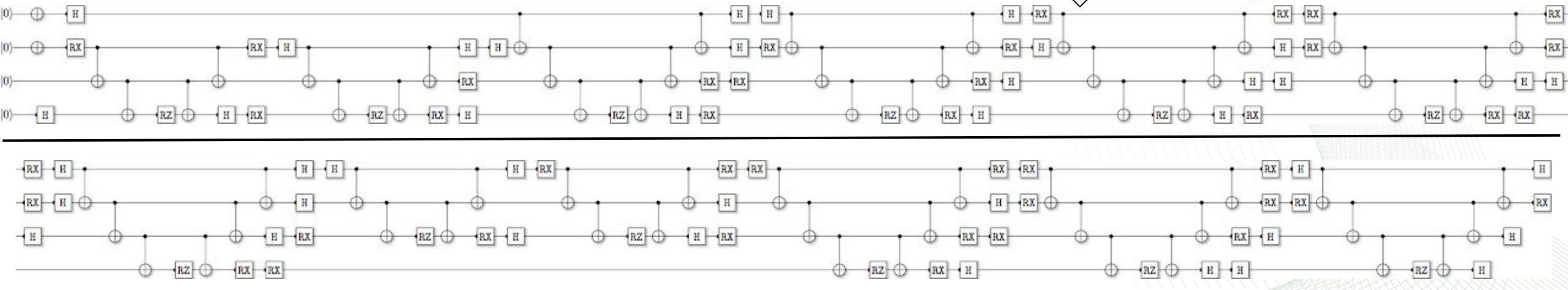
```
# Define the function we'd like to
# off-load to the QPU, here
# we're using a parameterized Factoring
# IR Generator
@xacc.qpu(accelerator='dwave')
def factor15(buffer):
    xacc(dwave-factoring, n=15)
```

produces

```
0 0 164.25;
1 1 168.25;
2 2 4;
3 3 -256.5;
0 1 100.25;
0 2 -14;
0 3 -224.5;
1 2 4;
1 3 -224.5;
2 3 32;
```

```
@xacc.qpu(accelerator=qpu) # or ibm, rigetti, etc...
def foo(buffer, t0, t1):
   xacc(uccsd, n_qubits=4, n_electrons=2)
   Measure(0,0)
```

produces



Python JIT Examples for D-Wave

```python
import xacc

xacc.Initialize()

# Get access to D-Wave QPU and
# allocate some qubits
dwave = xacc.getAccelerator('dwave')
qubits = dwave.createBuffer('q')

# Define the function we'd like to
# off-load to the QPU, here
# we're using a the QMI low-level language
@xacc.qpu(accelerator=dwave)
def f(buffer, h, j):
    qmi(0,0,h)
    qmi(1,1,h)
    qmi(0,1,j)

# Execute on D-Wave
f(qubits, 1., 2.)

# Print the buffer, this displays
# solutions and energies
print(qubits)

xacc.Finalize()
```

Get reference to the D-Wave Accelerator

Define the code you want to run, annotate it

Execute and post-process the results

```python
import xacc

xacc.Initialize()

# Get access to D-Wave QPU and
# allocate some qubits
dwave = xacc.getAccelerator('dwave')
buffer = dwave.createBuffer('q')

# Define the function we'd like to
# off-load to the QPU, here
# we're using a parameterized Factoring
# IR Generator
@xacc.qpu(accelerator='dwave')
def factor15(buffer):
    xacc(dwave-factoring, n=15)

# Factor 15 on the D-Wave
factor15(buffer)

# We have solutions as 0s and 1s
# decode that into our factors
xacc.analyzeBuffer(buffer)

# Print the factors
factors = buffer.getInformation('analysis-results')
xacc.info('Factors = ' + str(factors))

xacc.Finalize()
```

Thanks! Check out the project at:

https://github.com/eclipse/xacc

https://xacc.readthedocs.io

https://arxiv.org/abs/1710.01794

https://hub.docker.com/r/xacc

Email: xacc-dev@eclipse.org, mccaskeyaj@ornl.gov

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Looking ahead...

Quantum Parallel Processing

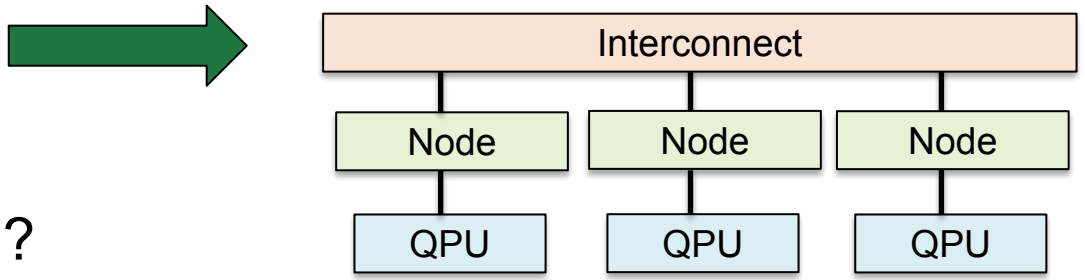
Hybrid ahead-of-time C++ compilation

Improved Python Integration

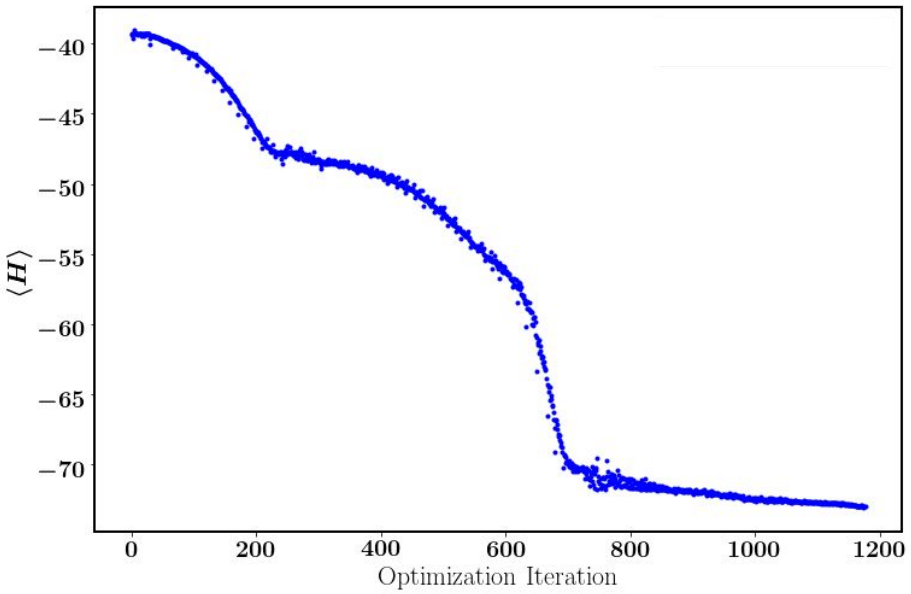
An Overall Integration Framework for Quantum Computing

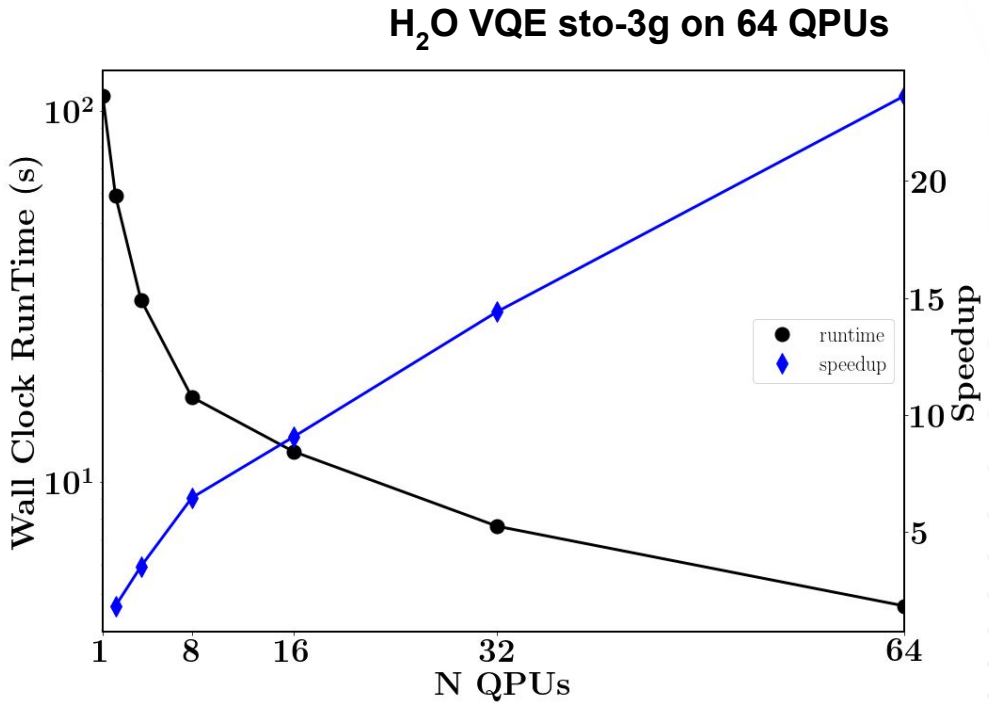
Future Quantum Parallel Processing with XACC

What if we had a compute system like this?



- How would you program it?
  - Popular MPI+X (X=OpenMP, CUDA, etc)
  - How about **MPI+XACC** programming Model?
  - **Shared vs Distributed** Memory QPP
- We've demonstrated this via an embarrassingly parallel distributed-memory VQE implementation





- **1086** Terms, 14 qubits
- **64 virtual QPUs**
- **28 VQE Parameters** - ~1200 Nelder Mead optimization steps
- **MPI All_Reduce** call to sum energies across cores
- Speedup and wall clock run-time based on simulation wall-clock time, rescale for QPU gate execution times

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Improved Python Integration

- Learn from CUDA Numba
- https://github.com/eclipse/xacc/issues/37
- Move away from string based kernel definitions
- Leverage
  - Python Decorators
  - Inspect Module
  - Custom XACC IR Antlr Grammar and Compiler
- Python users just annotate functions wrapping QPU code with `@qpu` and indicate target accelerator

framework code

```
import inspect

class qpu(object):
    def __init__(self, *args, **kwargs):
        self.args = args
        self.kwargs = kwargs
        return
    def __call__(self, f):
        def wrapped_f(*args, **kwargs):
            src = inspect.getsource(f)
            qpu = xacc.getAccelerator(self.kwargs['accelerator'])
            buf = qpu.createBuffer('q')
            program = xacc.Program(qpu, src)
            program.build()
            kernel = program.getKernels()[0]
            kernel.execute(buf, *args)
            return buf
        return wrapped_f
```

user code

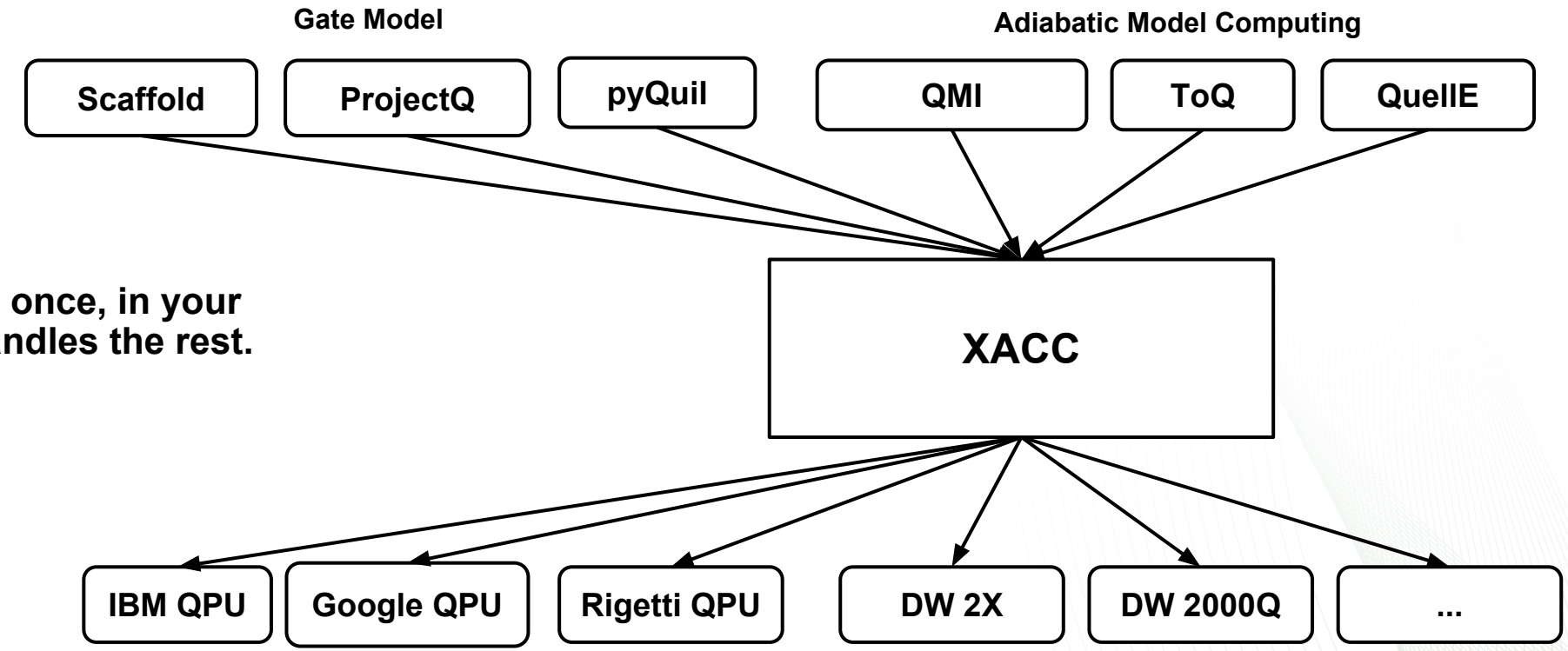
```
@qpu(accelerator='tnqvm') # or ibm, rigetti, etc...
def foo(theta):
   X(0)
   RY(theta, 1)
   CNOT(1, 0)
   Measure(0,0)
   return

results = foo(np.pi/3.)
print(results.getMeasurementBitStrings())
```

XACC Enabling Integration and Interoperability

- Language and Hardware interoperability
  - *"I prototyped this in X but want to run on Y"* - I've heard this a lot
  - Benchmarking will suffer without better software integration

Program quantum code once, in your language, and XACC handles the rest.

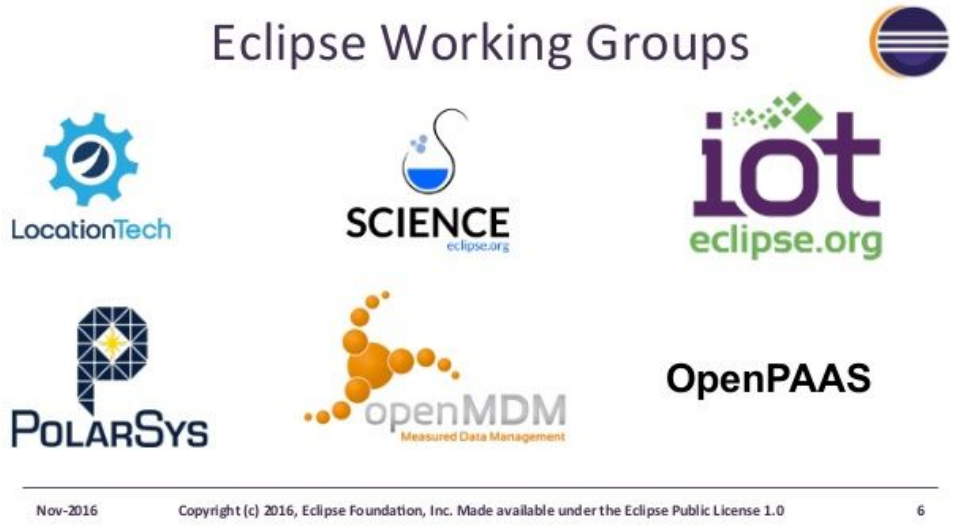


Eclipse XACC

- **Eclipse Foundation**
  - International organization
  - Eclipse IDE, 350 other open source projects
  - Working Group governance structure
    - Science, Location, IoT, etc...
  - IP tracking and management
  - IT Infrastructure
    - CI, GitHub, websites, email lists, etc…
  - ORNL is a member
- **XACC joined the Eclipse Foundation in 2017**
  - First C++ and quantum computing software project for Eclipse
  - Goal is research…
- The beginnings of a **Quantum Computing Software Working Group**
  - Quarterly virtual meetings (when possible)
  - Email mccaskeyaj@ornl.gov if interested in participating

OAK RIDGE National Laboratory

eclipse



Libraries and Applications built on XACC - XACC-VQE

```
$ xacc-vqe -f observable.hpp -t vqe -a ansatz.hpp
```

- XACC designed to serve as foundation for libraries and applications.
- Application built on XACC for VQE
  - https://github.com/ornl-qci/xacc-vqe
- Library of compiler routines for VQE problems
  - **`pragma`** for observable coefficients
- Provides **`VQEProgram`** and **`FermionCompiler`** extensions
- **`xacc-vqe`** command-line executable
- Task-based architecture
  - compute-energy, vqe, diagonalize, etc.

```
#pragma vqe-coefficient 5.906709445
__qpu__ idTerm(AcceleratorBuffer b) {
}
#pragma vqe-coefficient -2.1433
__qpu__ x0x1(AcceleratorBuffer b) {
H 0
H 1
MEASURE 0 [0]
MEASURE 1 [1]
}
#pragma vqe-coefficient -2.1433
__qpu__ y0y1(AcceleratorBuffer b) {
RX(1.57078) 0
RX(1.57078) 1
MEASURE 0 [0]
MEASURE 1 [1]
}
#pragma vqe-coefficient .21829
__qpu__ z0(AcceleratorBuffer b) {
MEASURE 0 [0]
}
```

```
__qpu__ ansatz(AcceleratorBuffer b,
               double t0) {
X 0
RY(t0) 1
CNOT 1 0
}
```

Higher-level programming and error mitigation

Deuteron binding energy via standard XACC Python API

```
import xaccvqe as vqe
from xaccvqe import qpu, PauliOperator
import xacc
import numpy as np

xacc.Initialize()
tnqvm = xacc.getAccelerator('tnqvm')
buffer = tnqvm.createBuffer('q',2)

ham = PauliOperator(5.906709445) + \
    PauliOperator({0:'X',1:'X'}, -2.1433) + \
    PauliOperator({0:'Y',1:'Y'}, -2.1433) + \
    PauliOperator({0:'Z'}, .21829) + \
    PauliOperator({1:'Z'}, -6.125)

@qpu.vqe(accelerator=tnqvm, observable=ham, optimizer='vqe-bayesopt', opt_params={'tol':1e-2})
def ansatz(buffer, initialTheta):
   X(0)
   Ry(initialTheta, 1)
   CNOT(1, 0)

ansatz(buffer, .5)

print(buffer.getInformation('vqe-energy'), buffer.getInformation('vqe-angles'))

xacc.Finalize()
```

Of note with this code sample

- Unified VQE API
- Problem programming at high-level, i.e. define Hamiltonian
- Custom ansatz generation using Python JIT
- Specify target Accelerator - IBM, Rigetti, TNQVM
- Built-in error mitigation (readout, arxiv:1612.02058, extrap. arxiv:1611.09301)
- Specify mapping to physical qubits