Quantum Computer Programming, Compilation, and Execution with XACC

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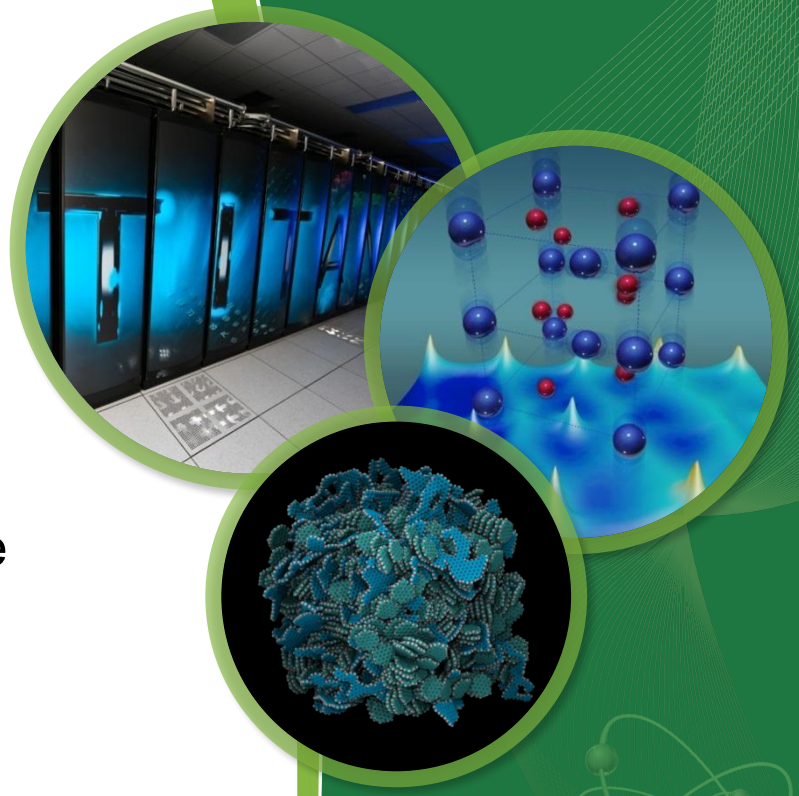
ORNL Software Expo Tutorial, May 2018



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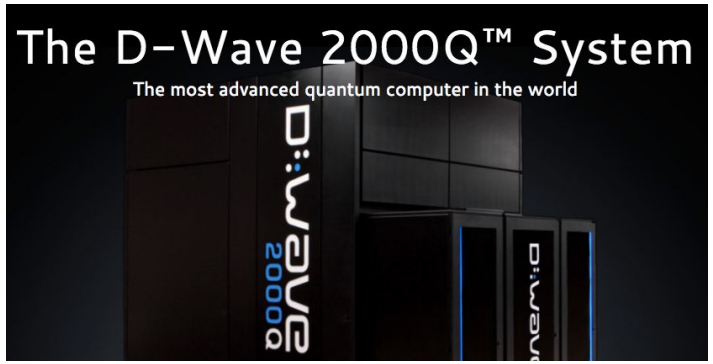
5 March 2018

Outline of Today's Tutorial...

- Quantum Computer Programming
- XACC - Motivation and Architecture
- Programming Interesting Hybrid Algorithms
  - Variational Quantum Eigensolver (VQE)
- Hands-on Demonstration
  - Compute ground state energy of H_2
  - Compute binding energy of deuteron (time permitting)



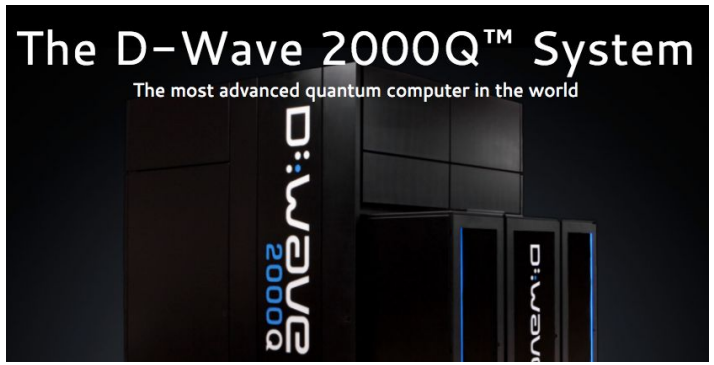
Logistics for the Demo

- Docker image with XACC, Openfermion, Psi4 and Jupyter Lab

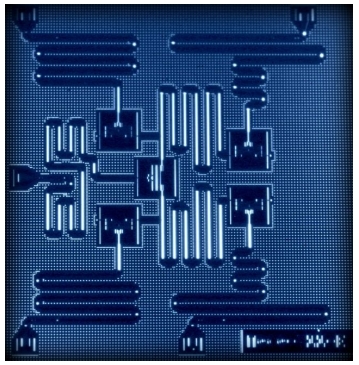
```
$ git clone https://github.com/eclipse/xacc
$ cd xacc/docker/expo_tutorial
$ docker-compose pull
$ docker-compose up -d
```

Navigate to `localhost:9000` on your browser!

```
$ (after tutorial) docker-compose down
```

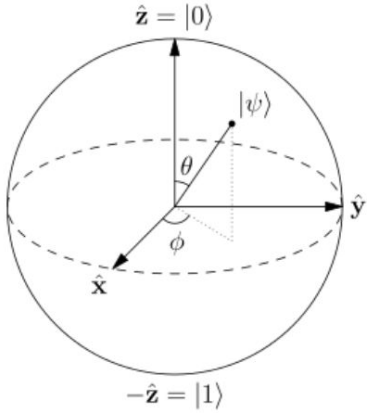


Quantum Computer Programming

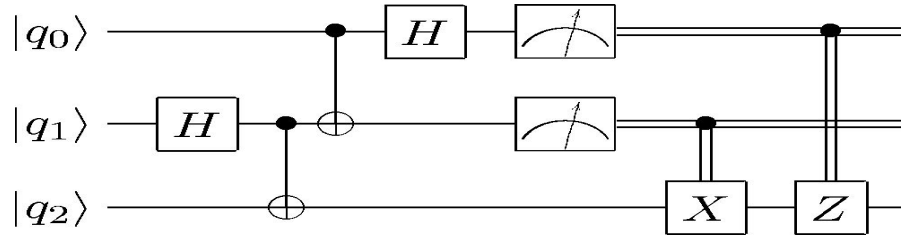


Gate Model

- Gates operate on qubits, modify qubit state
- Common gates are Rotations, entangling gates, and superposition gates
- Measure!

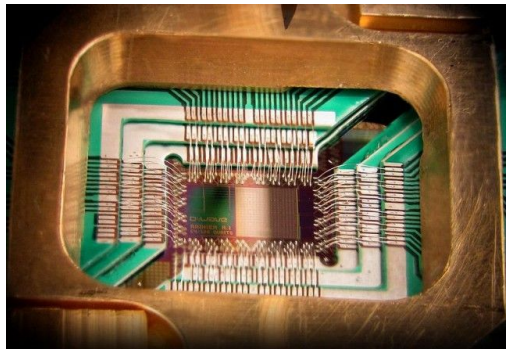



```
X(qreg[0]);
H(qreg[1]);
CNOT(qreg[1],qreg[2]);
CNOT(qreg[0],qreg[1]);
H(qreg[0]);
cbit c1 = MeasZ(qreg[0]);
cbit c2 = MeasZ(qreg[1]);
```



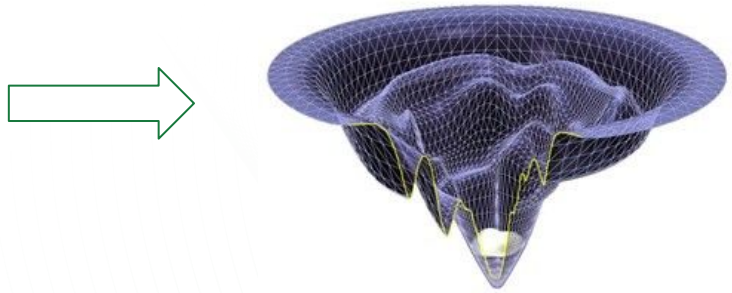
Quantum Annealing Model

- Encode problem into energy landscape - h_i and J_{ij}



$$E(x_1,\ldots,x_N) = \sum_{i=1} h_i\ x_i + \sum_{i<j=1}^{N} J_{ij}\ x_i x_j$$

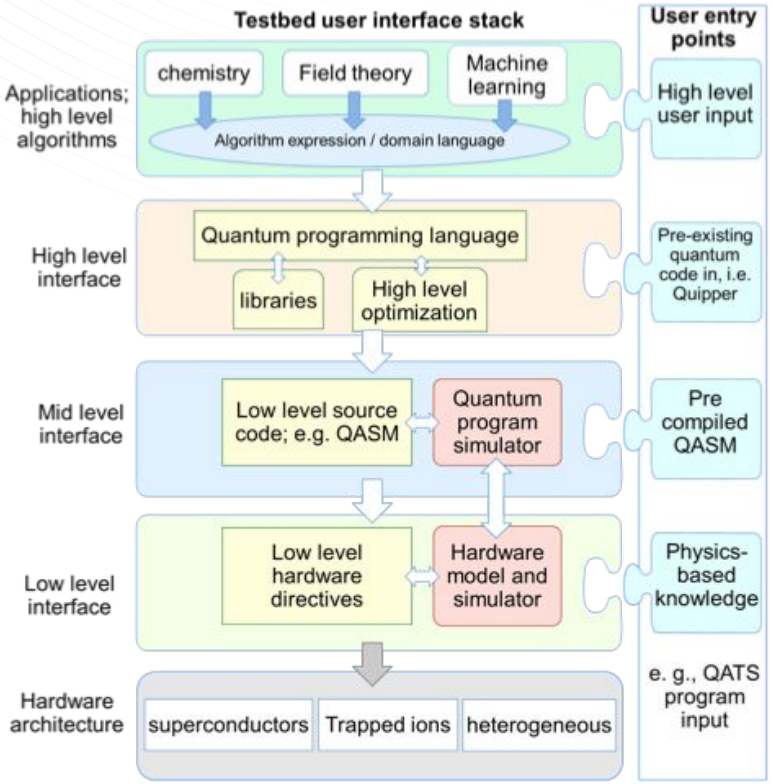
```
0 0 20;
1 1 50;
2 2 60;
4 4 50;
5 5 60;
6 6 -160;
1 4 -1000;
2 5 -1000;
0 4 -14;
0 5 -12;
0 6 32;
1 5 68;
1 6 -128;
2 6 -128;
```



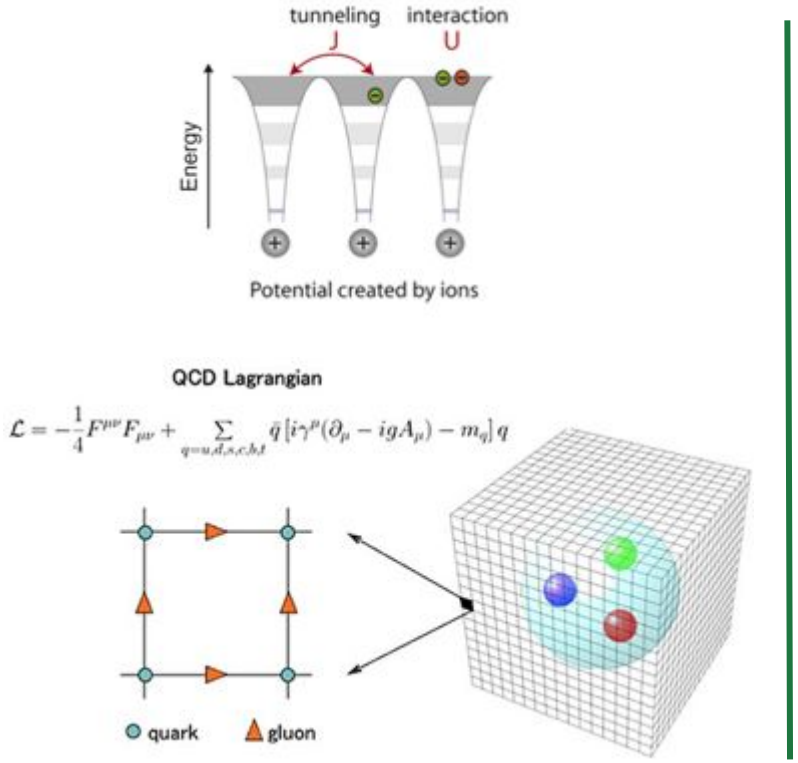
Quantum Software Efforts at ORNL

- What is driving ORNL quantum programming efforts?

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



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



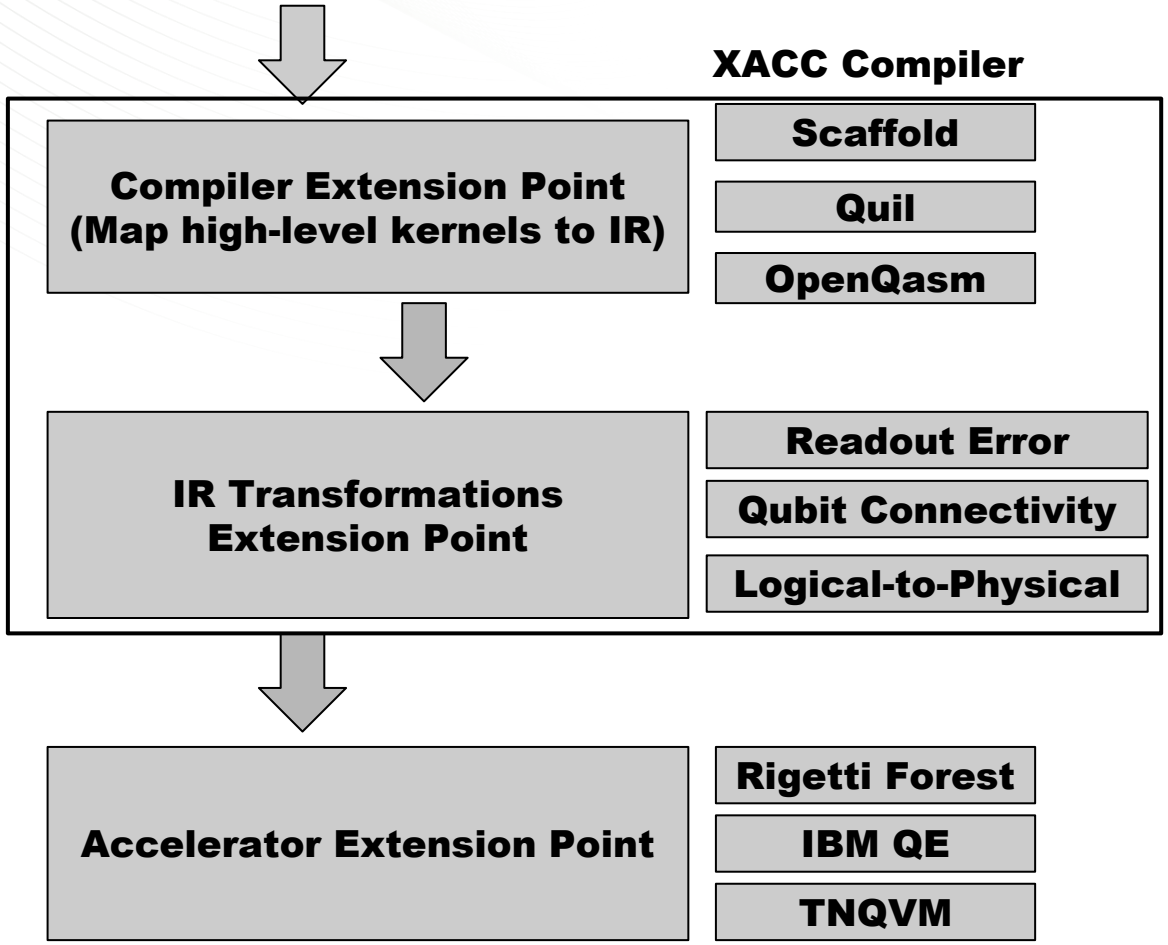
ORNL Programming Requirements

- Anticipation of ORNL Post-Exascale Computing
  - treat QPUs as accelerators
- MIQASA benchmarking across QPU hardware types
  - enable hardware-agnostic programming
- HDAQDS execution across QPU types and high-level program expression
  - extensibility in compilation techniques

Quantum Programming with XACC

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

```
__qpu__ quantum_kernel_foo(AcceleratorBuffer
qubit_register, Param p1, …, Param pN);
```



XACC:

- Open-source at https://github.com/eclipse/xacc
- Familiar API and model
  - OpenCL-like, hardware agnostic
- Key Abstractions
  - Kernels
  - Compilers
  - Intermediate Representation
  - Accelerators
- OSGI C++ Plugin Architecture (Python API available)

```
// 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.execute(buffer, theta);
```

XACC Model

Quantum Kernels

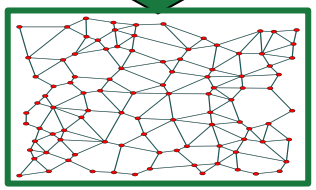
XACC - Heterogeneous CPU-QPU Programming Model

```
__qpu__ quantum_kernel_foo(AcceleratorBuffer qubit_register,
                           Param p1, …, Param pN);
```

Circuit

$$U_{kernel}|\psi_{register}\rangle$$

QUBO

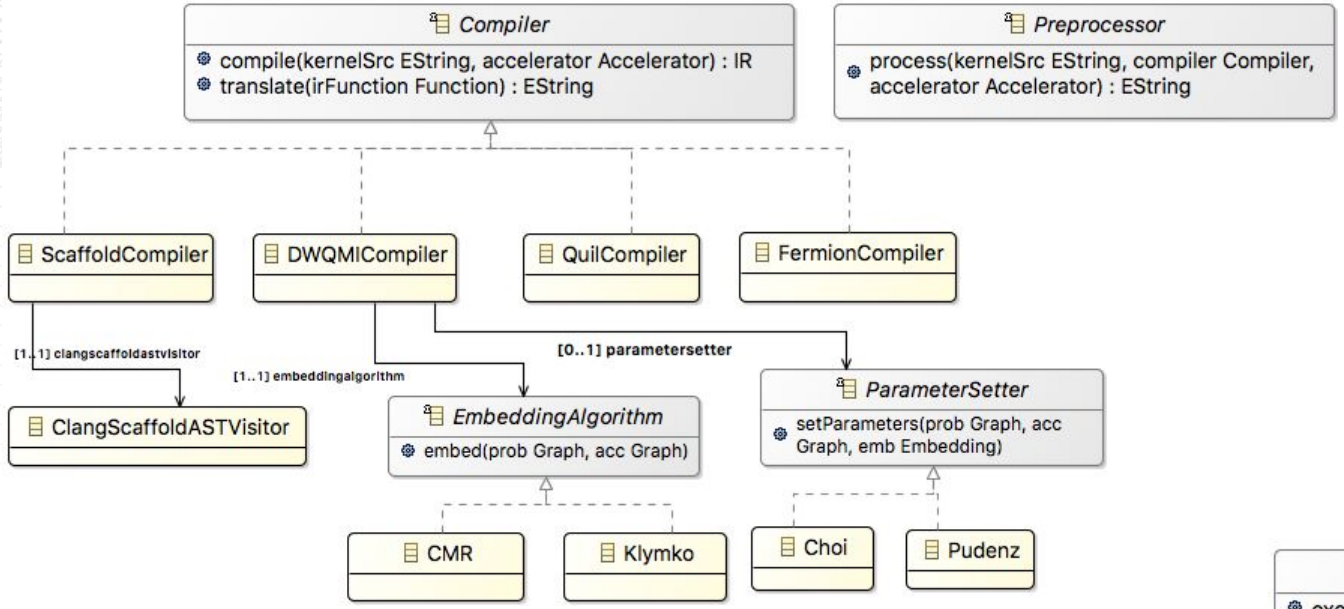


Example Gate Model Kernel written in Scaffold

```
__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__ 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.

Compilers and Accelerators



Compilers take source code and Accelerator, produce XACC IR

Compilers provide source-to-source translation capabilities

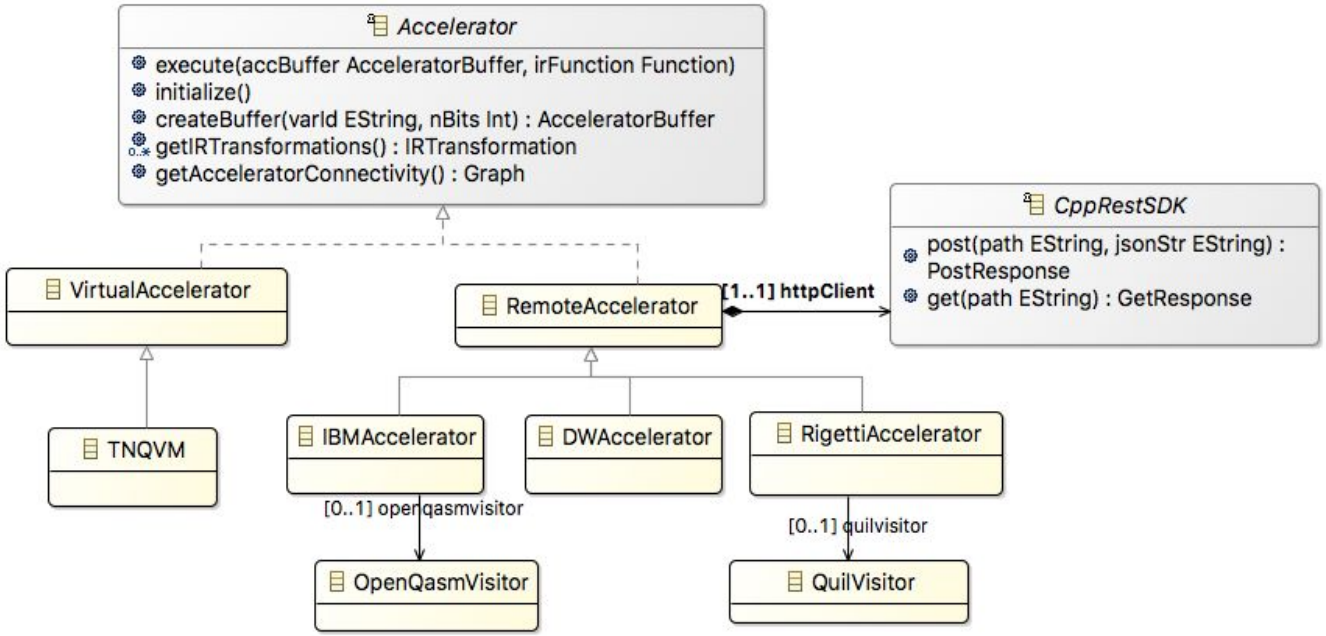
Extensible Preprocessor mechanism

Accelerators execute XACC IR

Can be simulators, physical QCs, remote or local

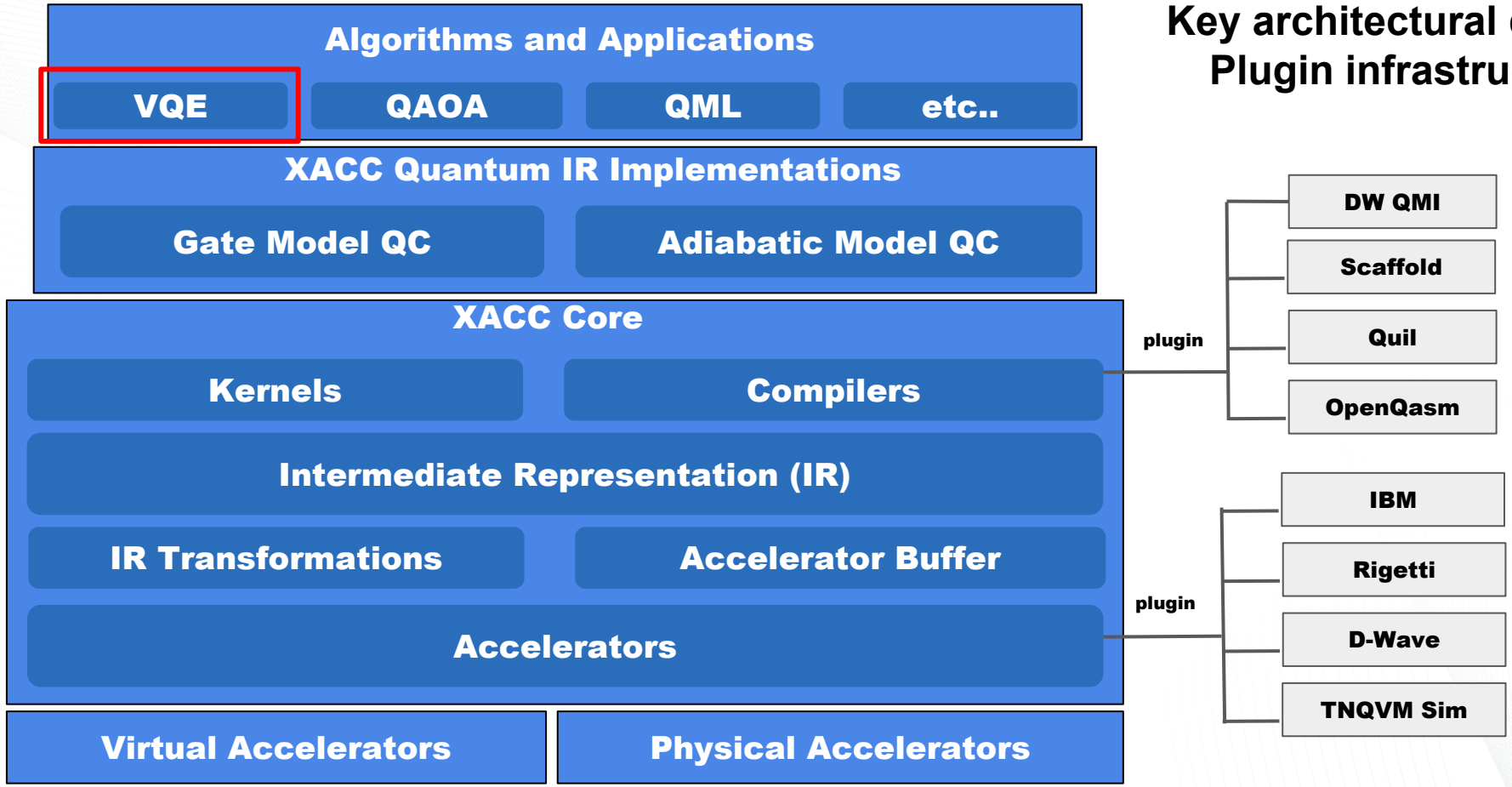
Remote Accelerators operate with HTTP Rest Client

Visitors walk IR, produce native code



Current XACC Application Stack

We'll be using this App for our Demo!

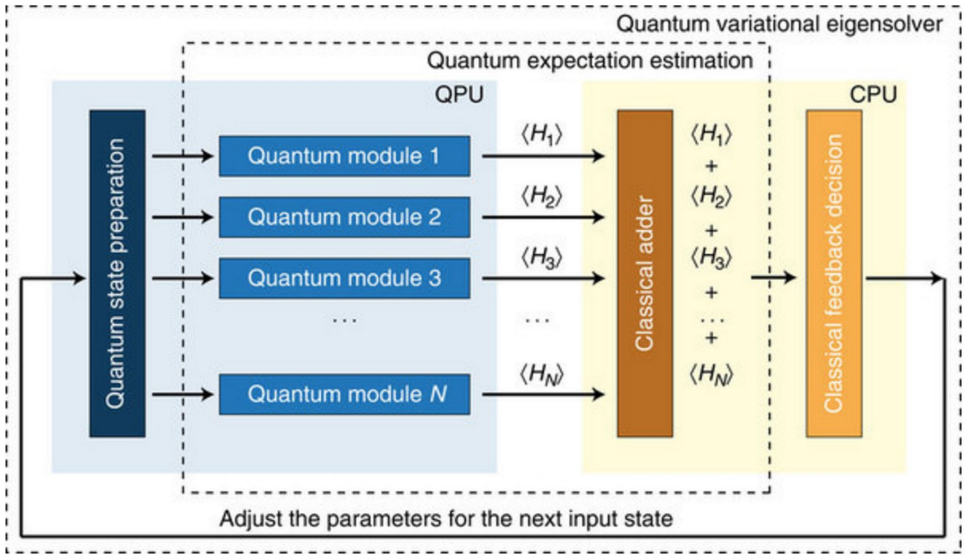


Key architectural design: Plugin infrastructure

XACC is the ONLY quantum programming model and framework that enables hardware-agnostic quantum programming, compilation, and execution. ORNL owns the only integration framework for quantum computing.

Variational Quantum Eigensolver (VQE)

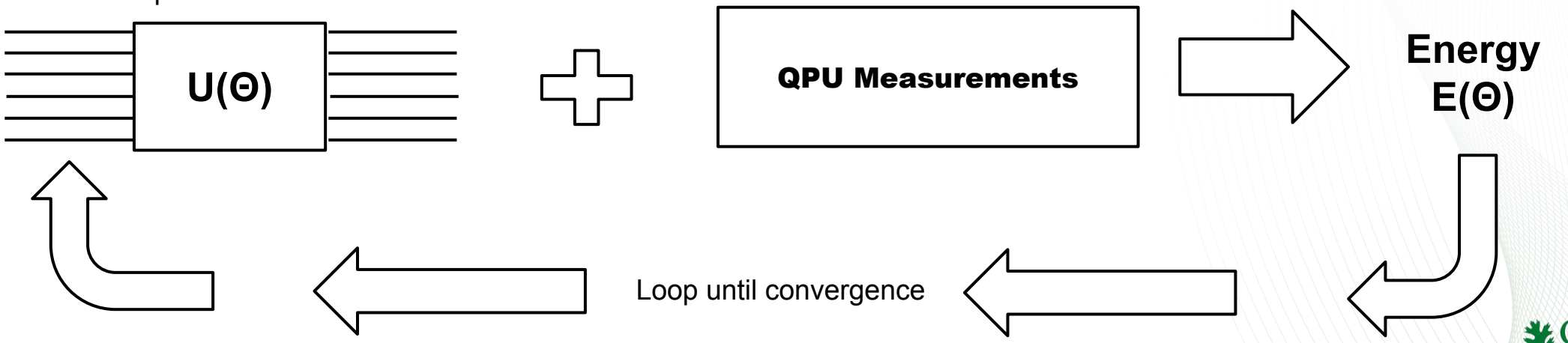
- Primary workhorse algorithm for research at ORNL
  - Compute eigenvalues of **H**
  - resistant to system level noise
  - ***Hybrid*** - leverages classical and quantum resources
  - Classical nonlinear optimization (search for ground state by optimizing classical parameters)



$$H = \sum_{p,q} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

compile!

Parameterized Circuit - Explores **H** Vector Space via controllable **Θ**



VQE Programming Steps

- Define your Hamiltonian
  - for H_2 / general quantum chemistry, we will use Openfermion and Psi4 quantum chemistry package
- Define your U(**Θ**)
  - H_2 - UCCSD auto generated by XACC
- Define classical optimization routine
  - We will use Nelder-Mead
- XACC handles compilation and execution on the Accelerator of your choice
  - TNQVM, IBM, Rigetti

$$H = \sum_{p,q} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

Psi4 provides an easy way to generate hpq, hpqrs

OpenFermion provides an easy to use FermionOperator data structure, which XACC can compile

XACC-VQE

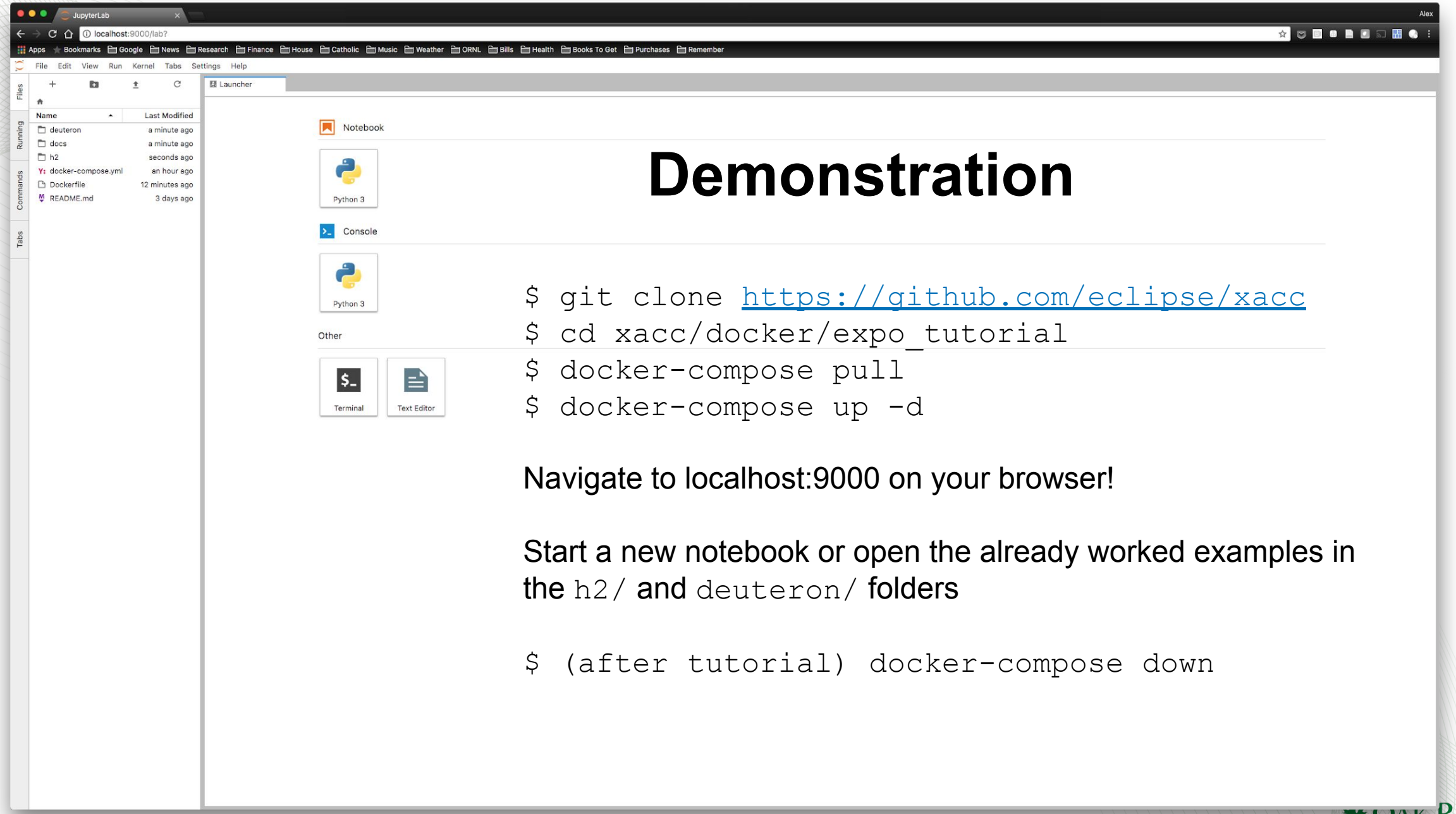
- Application built on XACC for VQE
  - https://github.com/ornl-qci/xacc-vqe
  - `xacc-vqe` binary executable
- Task-based architecture
  - compute-energy, vqe, diagonalize, etc.
- 2 API functions in Python
  - `compile(), execute()`
  - Both take as input a representation of the problem Hamiltonian
  - execute kwargs
    - ansatz, n-electrons, task, accelerator, etc...

```
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)

src = """__qpu__ ansatz(AcceleratorBuffer, double t0) {
X 0
RY(t0) 1
CNOT 1 0
}"""
ansatz = xacc.Program(qpu,src).getKernel('f').getIRFunction()

minEnergy = vqe.execute(ham, **{'ansatz':ansatz, 'accelerator':'ibm', \
                                'task':'vqe', 'n-qubits':12, \
                                'error-mitigation':['correct-readout-errors'], \
                                'qubit-map':[10,11]}).energy
```

```
ibmqx5Result = vqe.execute(H_f, **{
    'task':'compute-energy',
    'vqe-params':str(tnqvmResult.angles[0]), 'ansatz':statePrep,
    'accelerator':accelerator, 'qubit-map':[10,9],
    'error-mitigation':['correct-readout-errors']
    })
print('E = ', ibmqx5Result.energy)
```



Demonstration

```
$ git clone https://github.com/eclipse/xacc
$ cd xacc/docker/expo_tutorial
$ docker-compose pull
$ docker-compose up -d
```

Navigate to localhost:9000 on your browser!

Start a new notebook or open the already worked examples in the `h2/` and `deuteron/` folders

```
$ (after tutorial) docker-compose down
```

Accelerator Configuration

H2.ipynb | root@03a1314e

```
root@03a1314ef7dc:/# python -m pyxacc --help
usage: pyxacc.py [-h] [-c SET_CREDENTIALS] [-k API_KEY] [-u USER_ID] [--url URL] [-L] [--python-include-dir] [-b BRANCH]

XACC Framework Utility.

optional arguments:
  -h, --help            show this help message and exit
  -c SET_CREDENTIALS, --set-credentials SET_CREDENTIALS
                        Set your credentials for any of the remote Accelerators. (default: None)
  -k API_KEY, --api-key API_KEY
                        The API key for the remote Accelerators. (default: None)
  -u USER_ID, --user-id USER_ID
                        The User Id for the remote Accelerators. (default: None)
  --url URL             The URL for the remote Accelerators. (default: None)
  -L, --location        Print the path to the XACC install location. (default: False)
  --python-include-dir  Print the path to the Python.h. (default: False)
  -b BRANCH, --branch BRANCH
                        Print the path to the XACC install location. (default: master)
root@03a1314ef7dc:/# python -m pyxacc -c ibm -k YOUR_API_KEY
```

IBM Credentials

H2.ipynb | root@03a1314e

```
root@03a1314ef7dc:/# python -m pyxacc --help
usage: pyxacc.py [-h] [-c SET_CREDENTIALS] [-k API_KEY] [-u USER_ID] [--url URL] [-L] [--python-include-dir] [-b BRANCH]

XACC Framework Utility.

optional arguments:
  -h, --help            show this help message and exit
  -c SET_CREDENTIALS, --set-credentials SET_CREDENTIALS
                        Set your credentials for any of the remote Accelerators. (default: None)
  -k API_KEY, --api-key API_KEY
                        The API key for the remote Accelerators. (default: None)
  -u USER_ID, --user-id USER_ID
                        The User Id for the remote Accelerators. (default: None)
  --url URL             The URL for the remote Accelerators. (default: None)
  -L, --location        Print the path to the XACC install location. (default: False)
  --python-include-dir  Print the path to the Python.h. (default: False)
  -b BRANCH, --branch BRANCH
                        Print the path to the XACC install location. (default: master)
root@03a1314ef7dc:/# python -m pyxacc -c rigetti -k YOUR_API_KEY -u YOUR_USER_ID
```

Rigetti Credentials

If you would like to run on Rigetti Forest or IBM Quantum Experience, go to their respective sites and request free access.

https://quantumexperience.ng.bluemix.net/
https://www.rigetti.com/forest

Open a Terminal in the JupyterLab instance and run the commands to left to register your credentials with XACC

Otherwise, default Accelerator for this Demo will be the TNQVM tensor network simulator!

The Binding Energy of Deuteron

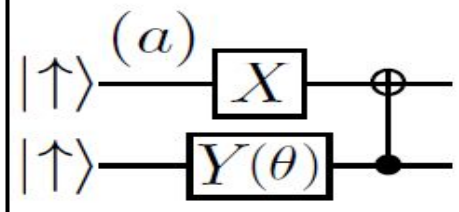
- Pionless EFT, discrete variable representation, HO basis, consider N=2,3, Jordan-Wigner
- We use variational quantum eigensolver (VQE) (over the cloud) method to identify the ground eigenstate (**arxiv:1801.03897)**

Deuteron N=2 Hamiltonian

$$H_2 = 5.906709I + 0.218291Z_0 - 6.125Z_1 - 2.143304\,(X_0X_1 + Y_0Y_1)$$

State Preparation Ansatz

$$U(\theta) \equiv e^{\theta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right)} = e^{i\frac{\theta}{2}(X_0Y_1 - X_1Y_0)}$$




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

```
#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]
}
#pragma vqe-coefficient -6.125
__qpu__ z1(AcceleratorBuffer b) {
MEASURE 1 [0]
}
```

Deuteron - Higher-level programming and error mitigation

Deuteron binding energy via standard XACC Python API

```
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)

src = """__qpu__ ansatz(AcceleratorBuffer, double t0) {
X 0
RY(t0) 1
CNOT 1 0
}"""
ansatz = xacc.Program(qpu,src).getKernel('f').getIRFunction()

minEnergy = vqe.execute(ham, **{'ansatz':ansatz, 'accelerator':'ibm', \
                                'task':'vqe', 'n-qubits':12, \
                                'error-mitigation':['correct-readout-errors'], \
                                'qubit-map':[10,11]}).energy
```

Of note with this code sample

- Unified VQE API
- Problem programming at high-level, i.e. define Hamiltonian
  - can define fermionic second quantized hamiltonians, XACC compiles to qubit representation
- Custom ansatz generation using Quill, Scaffold, OpenQasm, etc.
- Specify target Accelerator - IBM, Rigetti, TNQVM
- Built-in error mitigation (readout, arxiv:1612.02058, extrap. arxiv:1611.09301)
- Mapping to physical qubits (map to qubits with lowest two-qubit gate error rates)

...or how about program using OpenFermion and target IBM???

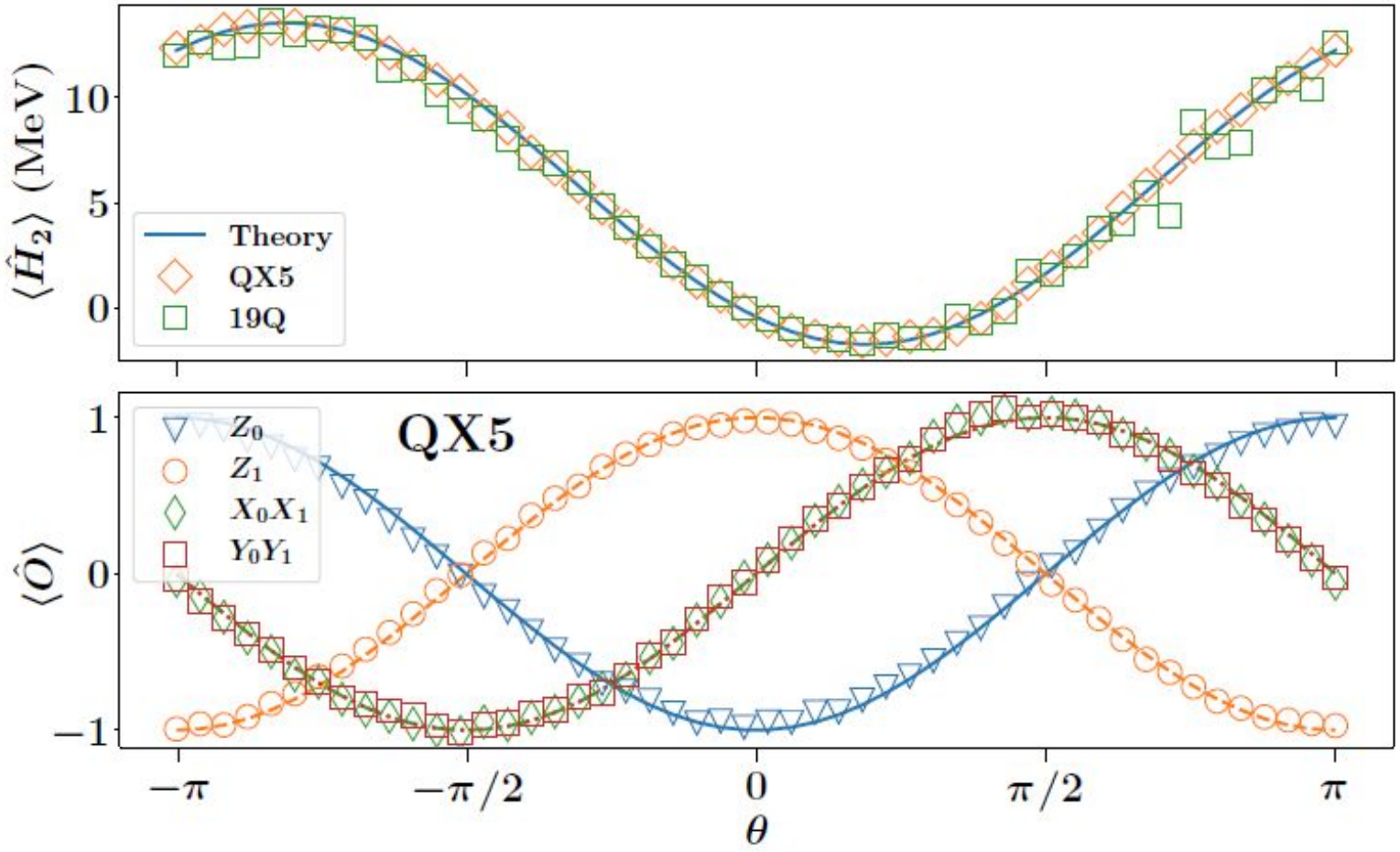
```
# Matrix elements
mat2=np.array([[ -0.43658111,  -4.28660705],
               [ -4.28660705,  12.25      ]])

# Create the Hamiltonian with OpenFermion
H_f = FermionOperator()
for i,j in [(0,0),(0,1),(1,0),(1,1)]:
    H_f += FermionOperator('{}^ {}'.format(i,j), mat2[i,j])
```

```
ibmqx5Result = vqe.execute(H_f, **{
    'task':'compute-energy',
    'vqe-params':str(tnqvmResult.angles[0]), 'ansatz':statePrep,
    'accelerator':accelerator, 'qubit-map':[10,9],
    'error-mitigation':['correct-readout-errors']
    })
print('E = ', ibmqx5Result.energy)
```

The Binding Energy of Deuteron - Results

Cloud Quantum Computing of an Atomic Nucleus - https://arxiv.org/abs/1801.03897



Top Panel

- This is the energy estimate of the theta-parameterized state
- Data taken on two processors, IBM and Rigetti

Bottom Panel

- The weighted sum of these terms gives the energy estimate
- These results yield a binding energy of 2.18 MeV based on fits of Luscher's formula

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

Funded by ORNL LDRD, DOE Testbed Pathfinder, DOE Quantum Algorithms Teams, DOE Early Career Research Program