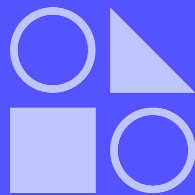


Quantum Machine Learning using Covalent

A QAOA application



Covalent.

Anna Hughes, PhD

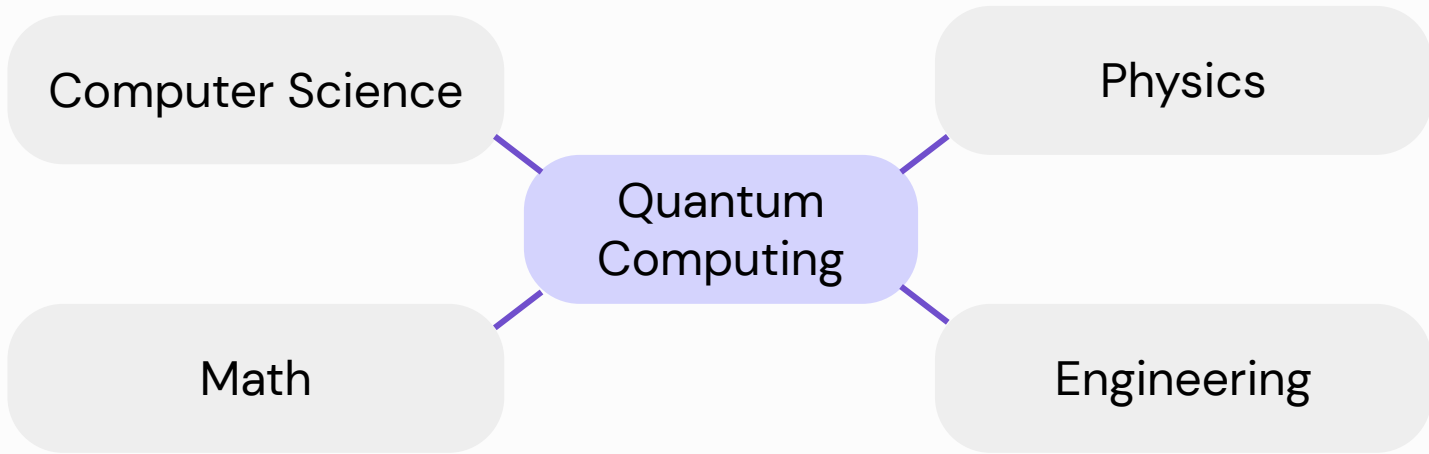
Quantum Software Engineer

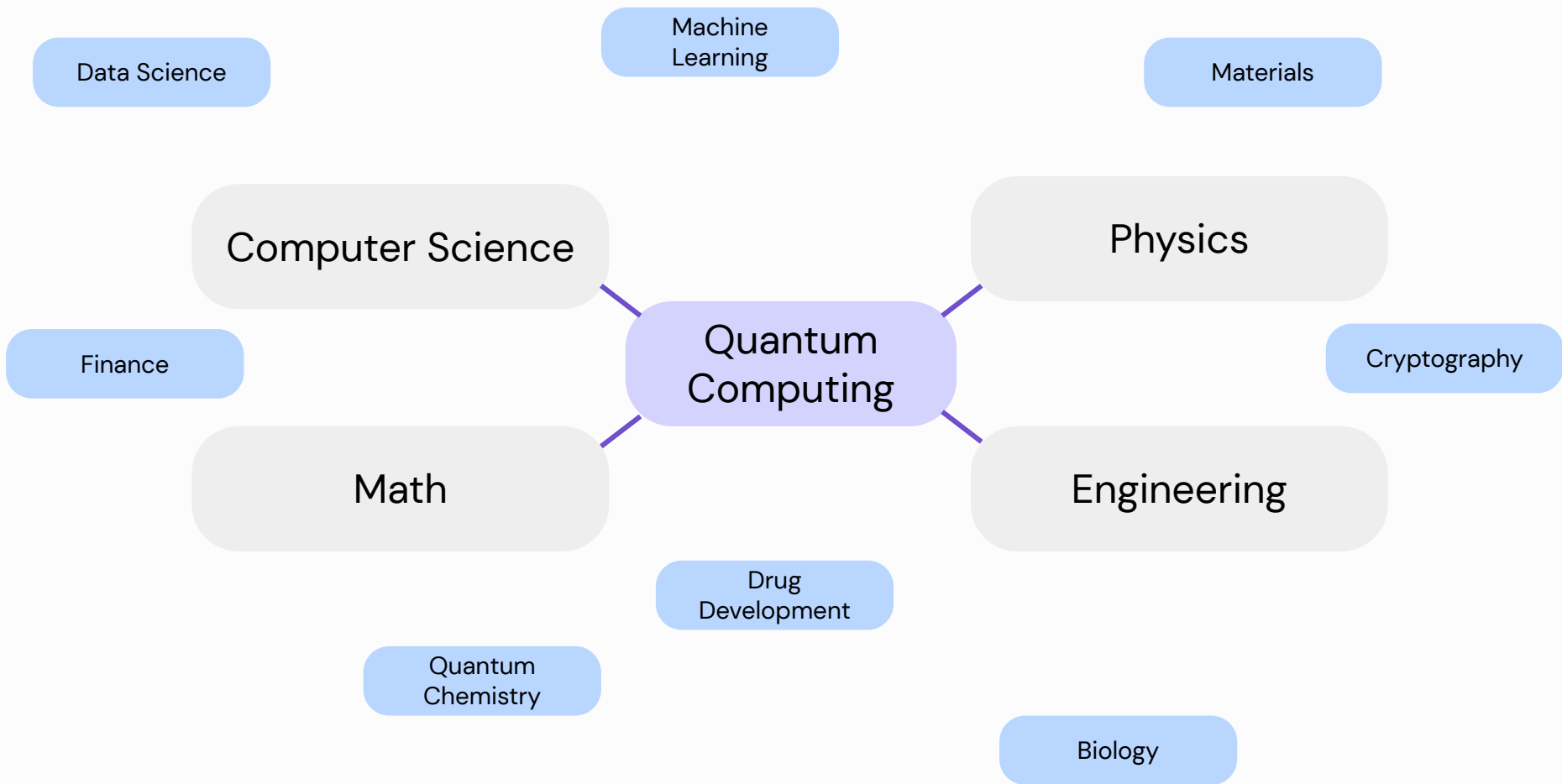
Some text to explain relevant role /
background

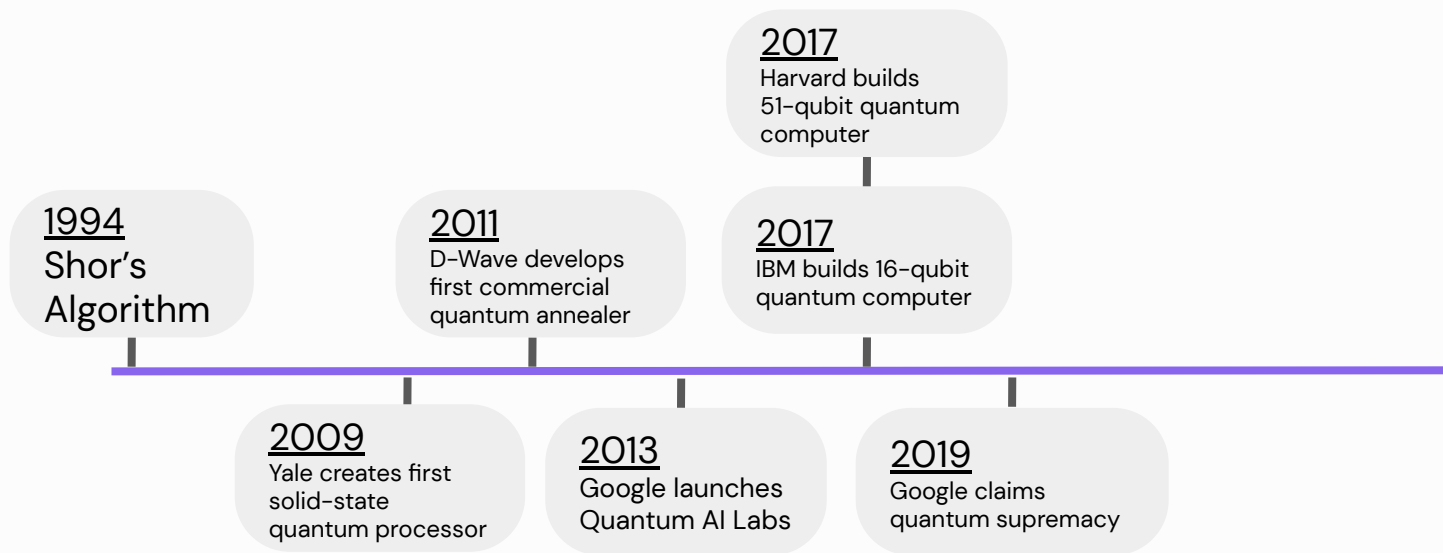


Introduction to Quantum Computing

Subheading

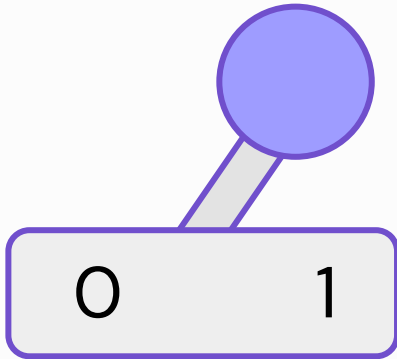






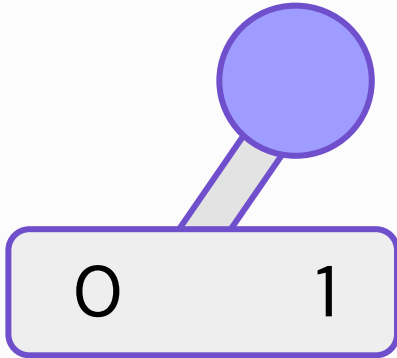
Classical Computers

Composed of **bits**, which can take on values of 0 or 1



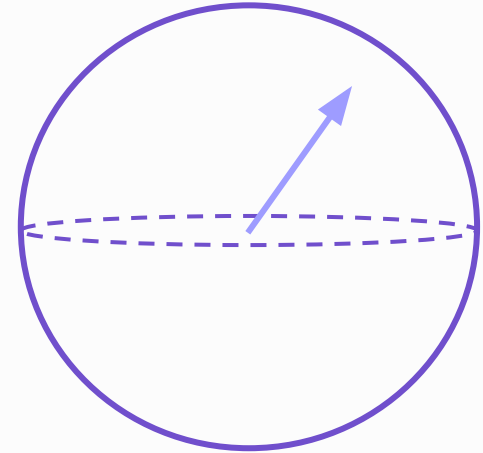
Classical Computers

Composed of **bits**, which can take on values of 0 or 1

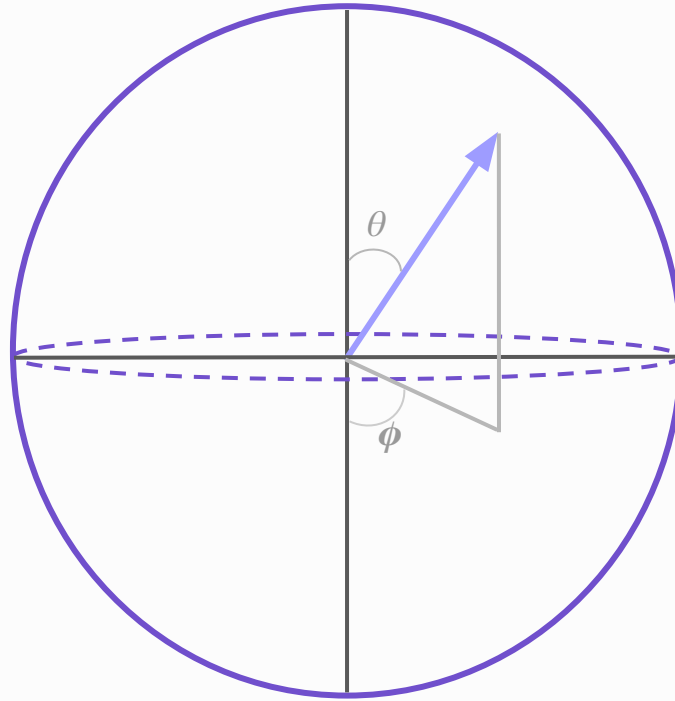


Quantum Computers

Composed of **qubits**, which can be in a superposition of 0 and 1

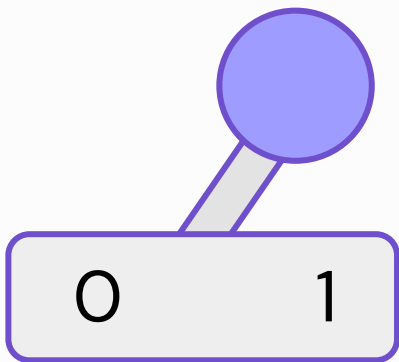


Bloch Sphere



Classical Computers

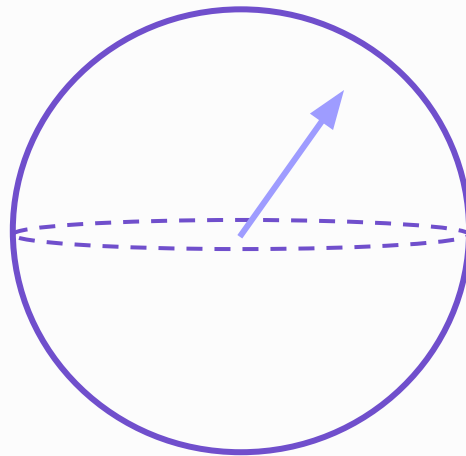
Composed of **bits**, which can take on values of 0 or 1



Deterministic measurements

Quantum Computers

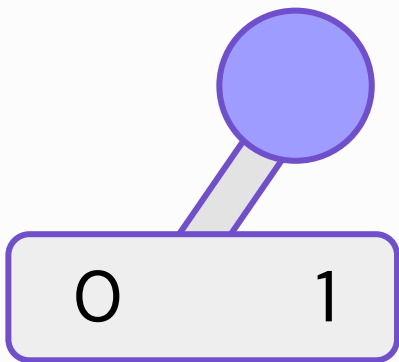
Composed of **qubits**, which can be in a superposition of 0 and 1



Probabilistic measurements

Classical Computers

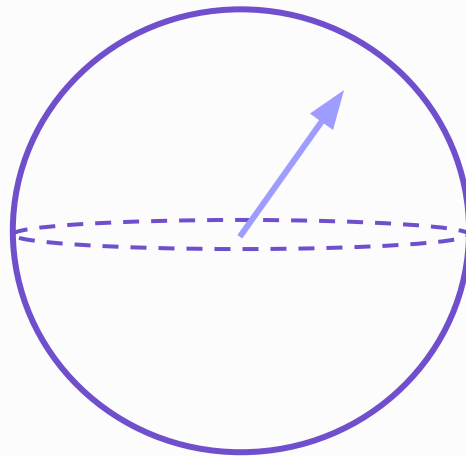
Composed of **bits**, which can take on values of 0 or 1



Deterministic measurements

Quantum Computers

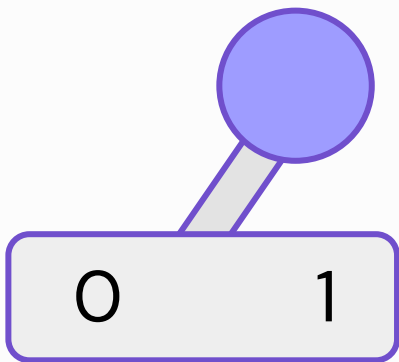
Composed of **qubits**, which can be in a superposition of 0 and 1



Probabilistic measurements

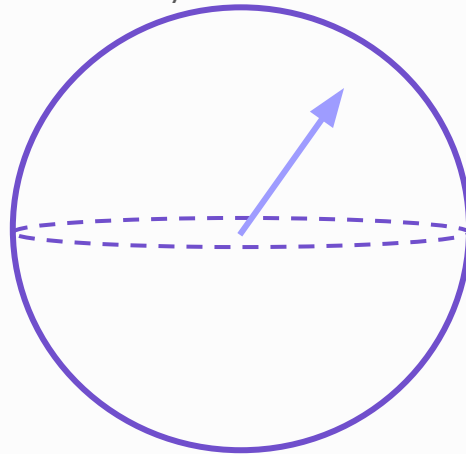
Classical Computers

If you have N bits, you have 2^N states that you can only execute 1 at a time (or in parallel)



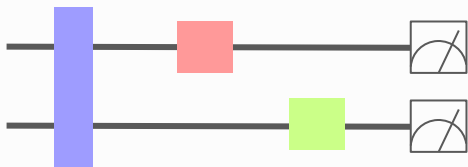
Quantum Computers

If you have N qubits, you can encode all 2^N components into one state simultaneously



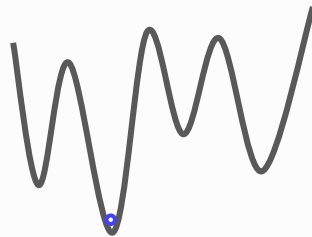
Probabilistic measurements

Types of Quantum Computers.



Gate-Based

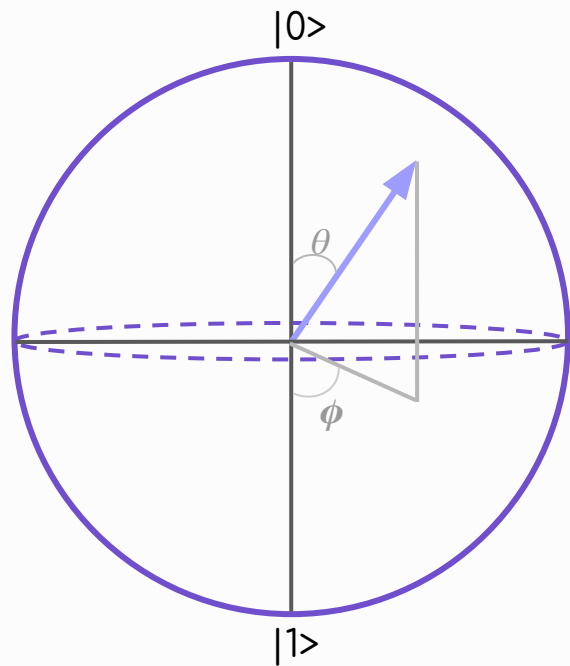
- Broad applications
- Apply gates, or circuit operations, to quantum state
-



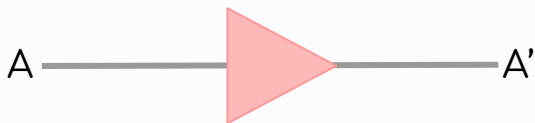
Quantum Annealers

- Can solve optimization problems: search an energy landscape for the lowest-energy solution
- Problem encoded as a Hamiltonian
-

Quantum Gates



○ Classical NOT Gate

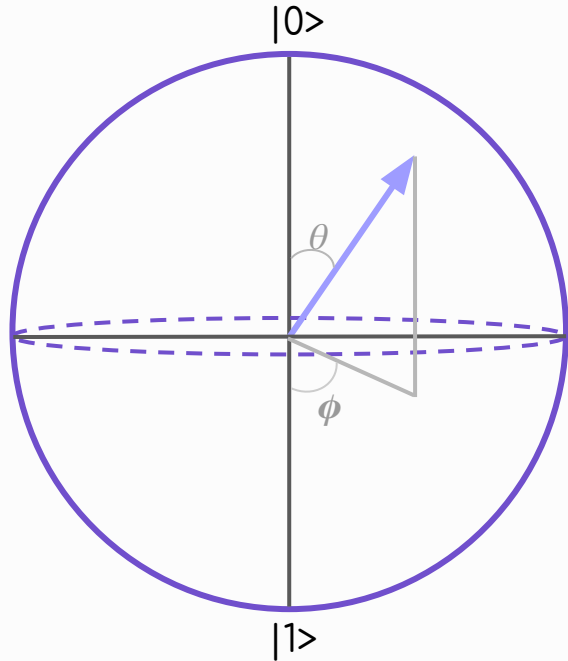


○ Pauli X Gate



$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Quantum Gates



- Pauli X Gate

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

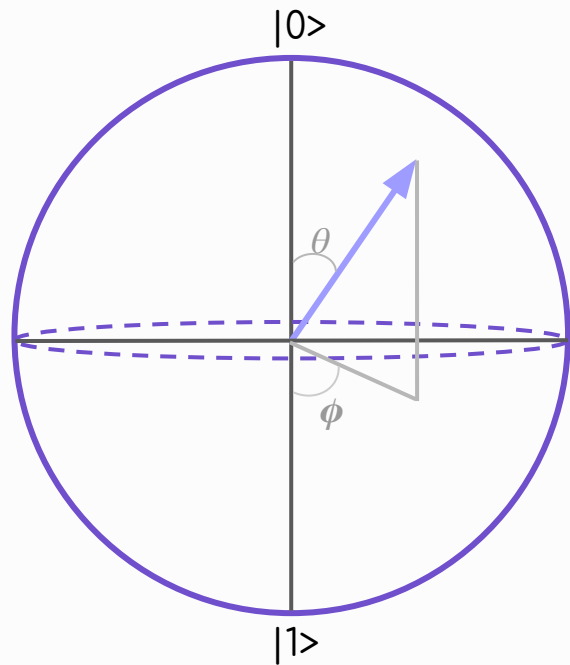
- Pauli Y Gate

$$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

- Pauli Z Gate

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Quantum Gates



- Pauli X Gate

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

- Pauli Y Gate

$$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

- Pauli Z Gate

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

covalent.xyz

- Hadamard Gate

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

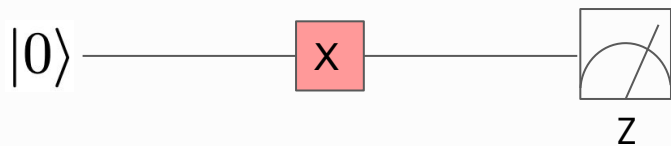
- Controlled NOT Gate

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

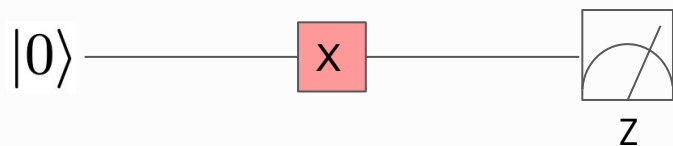
- Toffoli Gate

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Building a Quantum Circuit

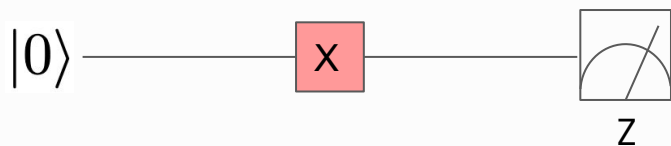


Building a Quantum Circuit



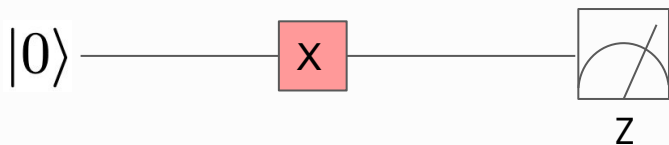
$$\begin{bmatrix} 1 \\ 0 \end{bmatrix} \longrightarrow \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Building a Quantum Circuit



$$\begin{array}{ccccc}
 \begin{bmatrix} 1 \\ 0 \end{bmatrix} & \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & \begin{bmatrix} 1 \\ 0 \end{bmatrix} & \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} & \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\
 |0\rangle & \sigma_x & |0\rangle & \langle 1 | \sigma_z | 1 \rangle & \\
 & = & & & \\
 & |1\rangle & & &
 \end{array}$$

Building a Quantum Circuit

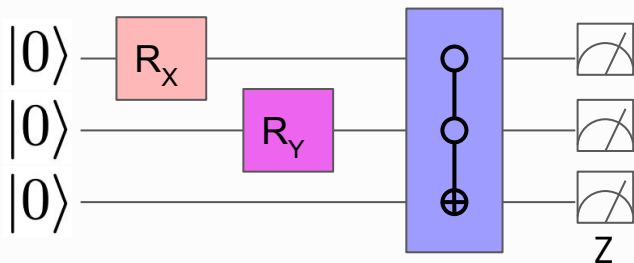


```
import pennylane as qml

dev1 = qml.device("default.qubit", wires=1)

@qml.qnode(dev1)
def circuit():
    qml.PauliY(wires=0)
    return qml.expval(qml.PauliZ(0))
```

Building a Quantum Circuit



```
import pennylane as qml

dev1 = qml.device("default.qubit", wires=3)

@qml.qnode(dev1)
def circuit(params):
    qml.RX(params[0], wires=0)
    qml.RX(params[0], wires=1)
    qml.CNOT(wires=[0,1])
    qml.CNOT(wires=[1,2])
    return qml.expval(qml.PauliZ(0)),
    qml.expval(qml.PauliZ(1)), qml.expval(qml.PauliZ(2))
```



Introduction to Quantum Machine Learning

Subheading

Machine Learning



A **model** is developed to describe and make predictions about data



Model **parameters** are tuned using a **training dataset**



The model is assessed by making predictions about a **test dataset**

Machine Learning



A **model** is developed to describe and make predictions about data

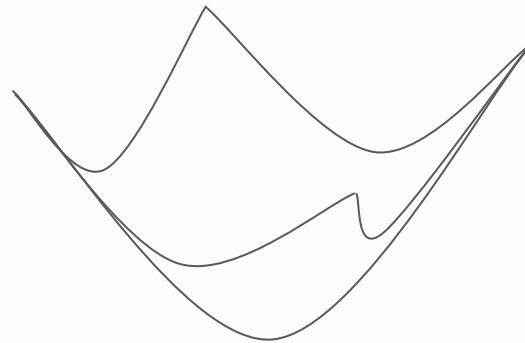


Model **parameters** are tuned using a **training dataset**



The model is assessed by making predictions about a **test dataset**

Optimizing a cost function

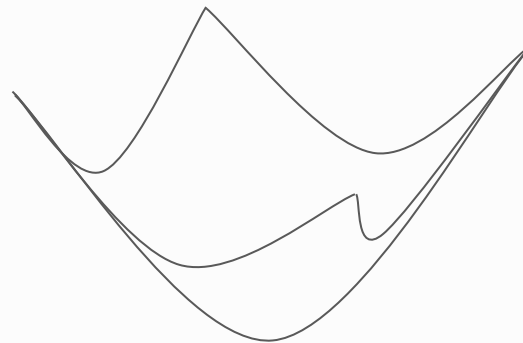


Machine Learning Example



A **model** is developed to describe and make predictions about data

Optimizing a cost function



Machine Learning Example



Overfitting.

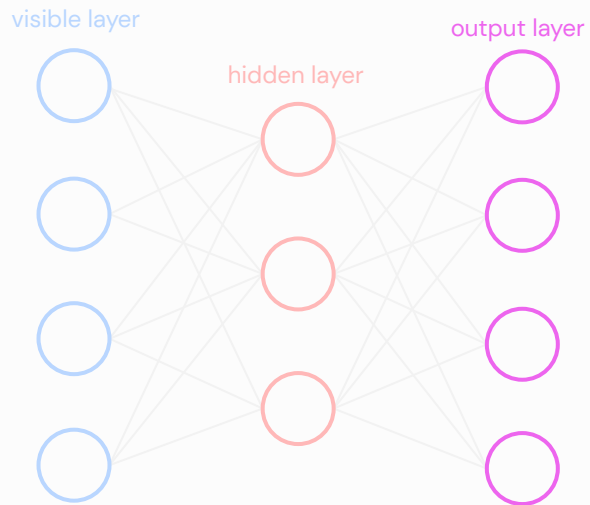
Era of high-throughput calculations. Running massive parallel jobs at scale.



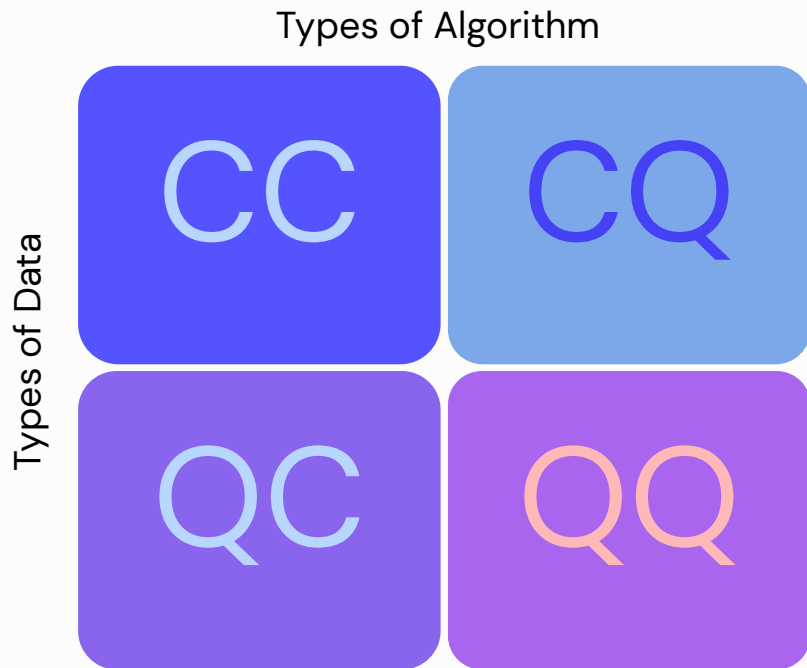
Underfitting.

High performance computing in the age of **rapid prototyping** and experimentation.

Neural Networks



Quantum Machine Learning



Quantum Machine Learning

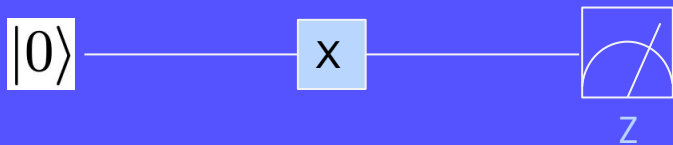
Types of Algorithm

Types of Data

CQ

classical data with
quantum algorithms

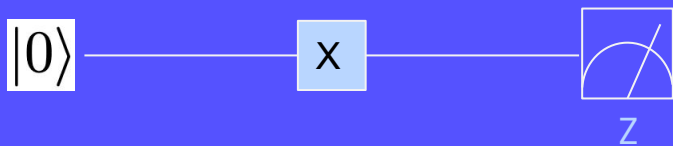
Parameterized Quantum Circuits



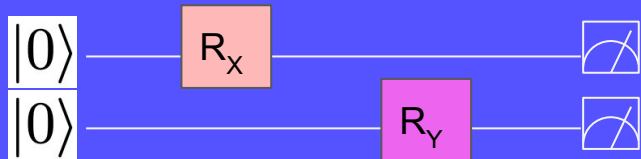
This circuit does not have tunable parameters



Parameterized Quantum Circuits



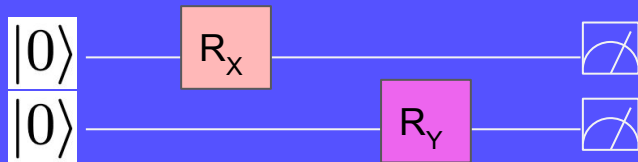
This circuit does not have tunable parameters



The input angles in R_x and R_y are tunable parameters



Parameterized Quantum Circuits



The input angles in R_x and R_y are tunable parameters

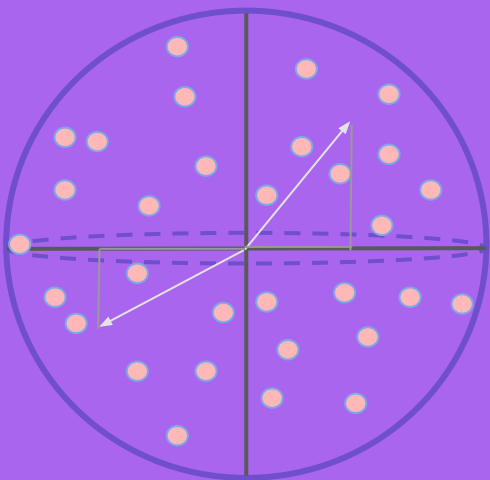
A quantum circuit with tunable parameters consists of unitary operations $U(\theta)$ performed on n qubits

Parameterized Quantum Circuits



Expressibility.

We want our quantum circuit to be able to span a wide subset of Hilbert Space!



Entanglement.

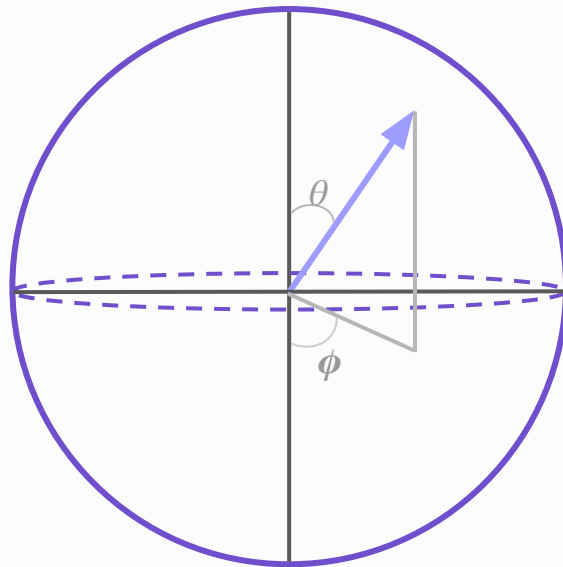
Entangled qubits are difficult to simulate using a classical simulator.

Parameterized Quantum Circuits



Expressibility.

We want our quantum circuit to be able to span a wide subset of Hilbert Space!

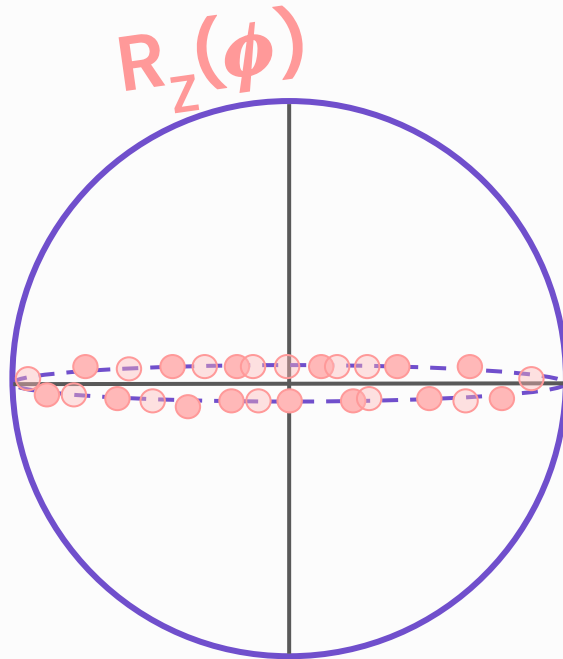


Parameterized Quantum Circuits



Expressibility.

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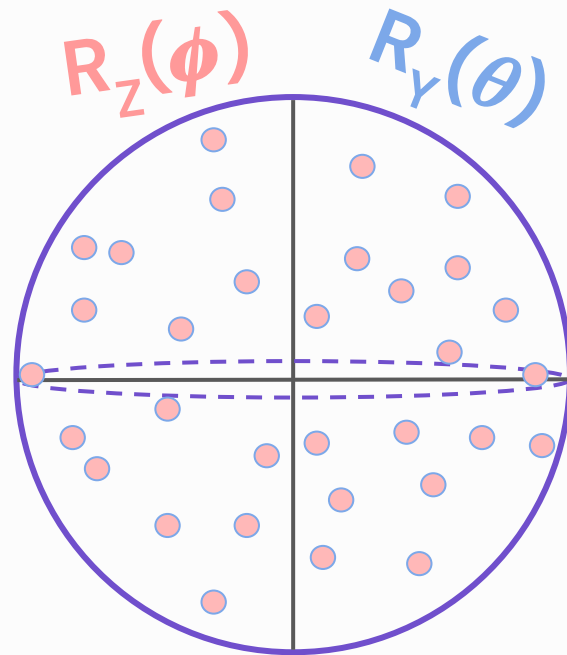


Parameterized Quantum Circuits



Expressibility.

We want our quantum circuit to be able to span a wide subset of Hilbert Space!

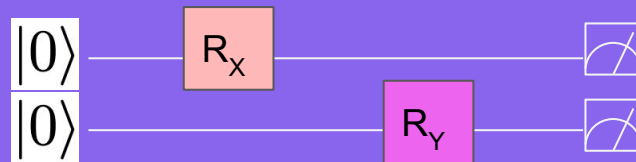


Parameterized Quantum Circuits

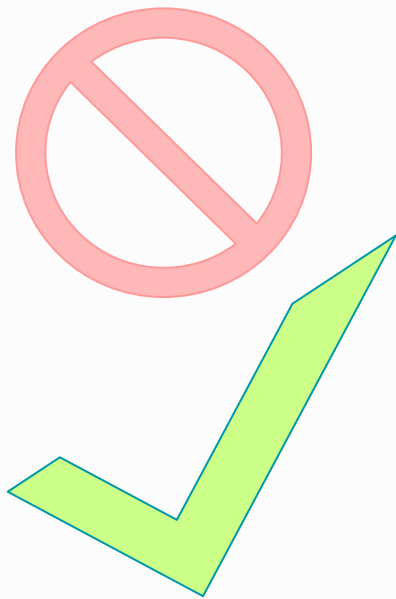


Entanglement •

Entangled qubits are difficult to simulate using a classical simulator.

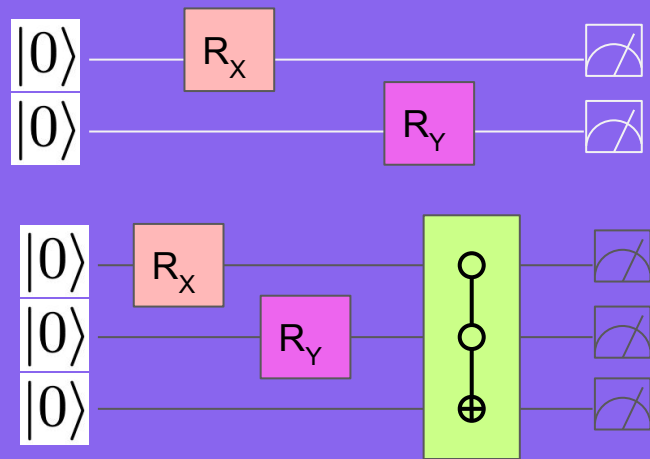


Parameterized Quantum Circuits



Entanglement

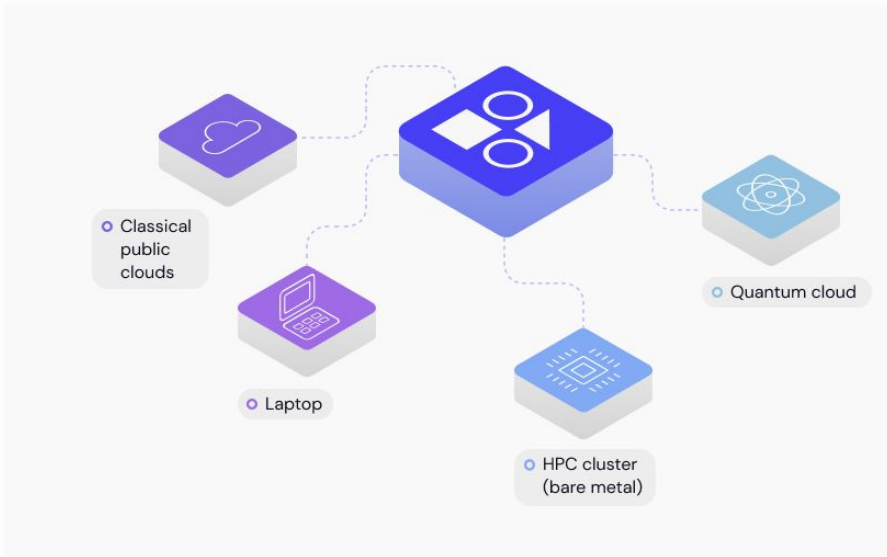
Entangled qubits are difficult to simulate using a classical simulator.



Covalent is an open source workflow orchestration platform for quantum and high performance computing

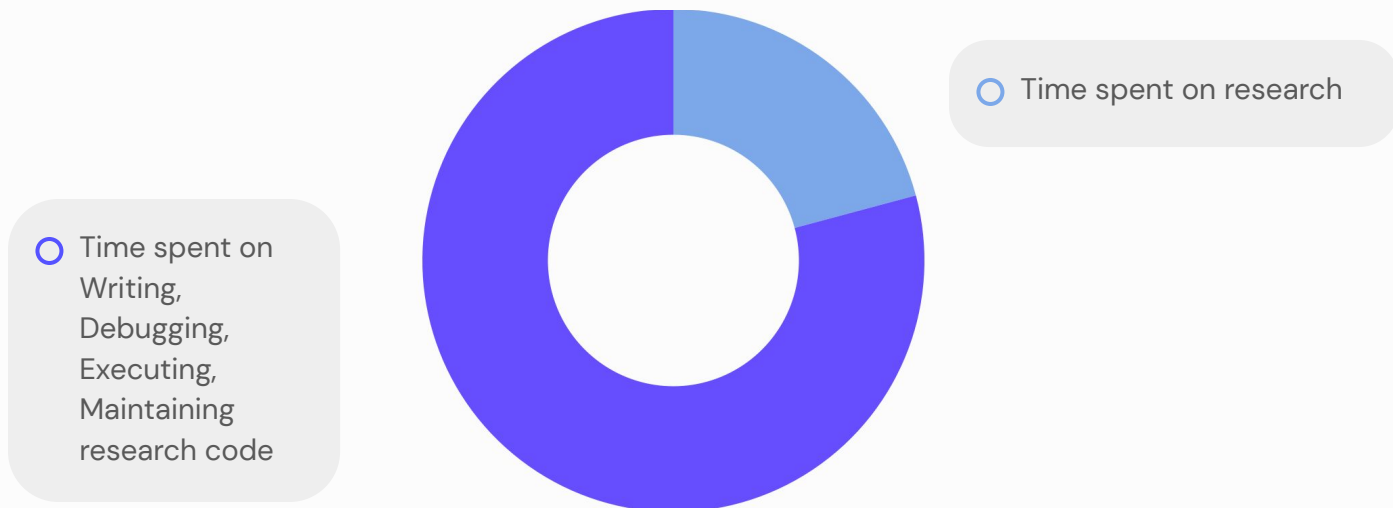
Covalent is designed to make your experiments:

- Modular
- Scalable
- Reproducible



Why does Covalent exist?

Computational research



Challenges.

Experimental-Organization



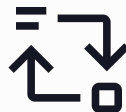
Manageability.

- Organize 1000s of experiments
- Experimental versioning of multiple runs
- Input/parameters logging for each run
- Checkpointing costly computations
- Job failure management
- Real time monitoring



Reproducibility.

- Environment saving/caching
- Hardware metadata caching
- Inputs/parameters logging
- Experiment dependant device setup

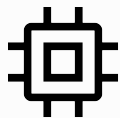


Shareability.

- Experiment organization
- Clear and intuitive code structure
- Reproducible experiment parameters and setup

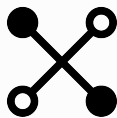
Challenges.

Computational



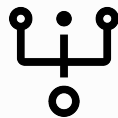
Hardware-potpourri.

Hybrid research / experiments.
Single experiment now contains
CPU+GPU+QPU+TPU



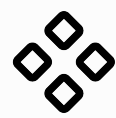
Interactive HPC.

High performance computing in
the age of rapid prototyping and
experimentation.



Distributed computation.

Era of high-throughput
calculations. Running massive
parallel jobs at scale.



Limited resource.

Long queue time, quantum
queues and Server-less HPC!

How Covalent can help.



Solution 1.

Hybrid research / experiments.
Single experiment now contains
CPU+GPU+QPU+TPU



Solution 2.

High performance computing in
the age of **rapid prototyping** and
experimentation.



Solution 3.

Era of high-throughput
calculations. Running massive
parallel jobs at scale.



Solution 4.

Long queue time, quantum queues
and **Server-less HPC!**



3. Real-time monitoring

Visual overview

Visualize and share your workflow to transfer knowledge as fast as possible

Status/Error updates

Get real time Updates on errors and completion

Checkpoints

Stores anything and everything automatically without a single line of code

Meta-data

Maintains details from environment to hardware used

Parameter

Never forget the hyper-parameters that worked

Interactive

Start/stop/manage your HPC jobs right from the UI

Beautiful and interactive UI

bring your workflows to life!



Where Covalent fits in the stack.



Ecosystem



Classical resources

- SLURM Executer
- AWS-Fargate Executer
- AWS-Batch Executer
- Azzure Executer Coming soon
- GCP Executer Coming soon
- Kubernetes Executer Coming soon

Many more



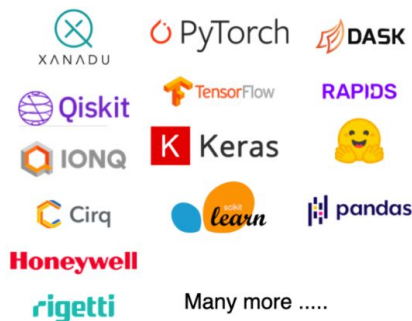
Quantum resources

- AWS-Braket-jobs Executer Coming soon
- Qiskit-Runtime Executer Coming soon

Many more

□ Or, Write your own !

Any and all package!



Many more

Language Support



There is more.

Pythonic
workflows

Automatic
checkpointing

Multiple language
support

Little-to-no
overhead

Customizable

Reproducibility

Code locally,
un anywhere



Intuitive
User-interface

Natively hybrid
workflows

Native
parallelization

Variety of
executors

Code
isolation

Parameter
caching

Cloud
Agnostic

Interactive
jobs

Start locally
and scale

Comparison table.

Languages.

- Python
- C / C++
- Julia*
- Bash

Executors.

- Local executors
- Slurm
- AWS*
- GCP*
- Azure*

*Roadmap item

Code.

○○○

○

```
1    # Transaction in Python
2    session.start_transaction()
3    order = { line_items : [ { item : 5, quantity: 6 } ] }
4    db.orders.insertOne( order, session=session );
```

Code.

○○○

○

```
1      # Transaction in Python
2
3      session.start_transaction()
4      order = { line_items : [ { item : 5, quantity: 6 } ] }
5      db.orders.insertOne( order, session=session );
6      for x in order.line_items:
7          db.inventory.update(
8              { _id : x.item },
9              { $inc : { number : -1 * x.quantity } },
10             session=session
11
12      session.start_transaction()
13
14
```

○○○

○

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1      # Transaction in Python
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```

Code.

○○○



```
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○○○



```
1      # Transaction in Python
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4      order = { line_items : [ { item : 5, quantity: 6 } ] }
5      db.orders.insertOne( order, session=session );
```

Code.

○○○



```
1 # Transaction in Python
2
3 session.start_transaction()
4 order = { line_items : [ { item : 5, quantity: 6 } ] }
5 db.orders.insertOne( order, session=session );
```

○○○



```
1 # Transaction in Python
2
3 session.start_transaction()
4 order = { line_items : [ { item : 5, quantity: 6 } ] }
5 db.orders.insertOne( order, session=session );
```

○○○



```
1 # Transaction in Python
2
3 session.start_transaction()
4 order = { line_items : [ { item : 5, quantity: 6 } ] }
5 db.orders.insertOne( order, session=session );
```

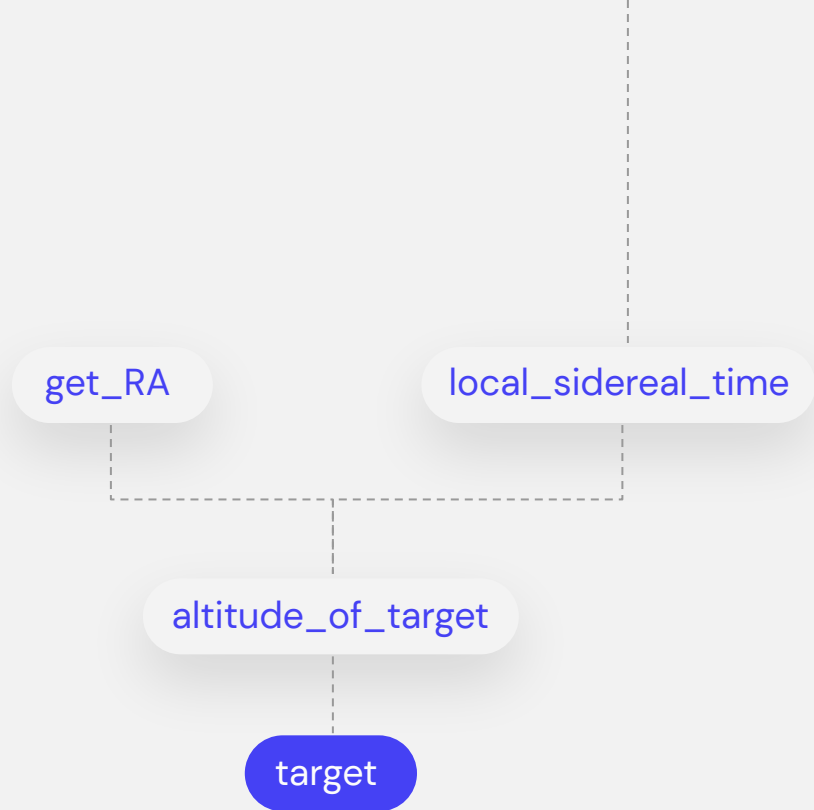
○○○



```
1 # Transaction in Python
2
3 session.start_transaction()
4 order = { line_items : [ { item : 5, quantity: 6 } ] }
5 db.orders.insertOne( order, session=session );
```

Components.

Diagram



Optimizing financial portfolios on superconducting and trapped ion quantum computers.

A combinatorial optimization problem arises whenever we are presented with a number of choices and we task ourselves with selecting the best choice. One example surfaces from a problem often posed by delivery companies: “given a set of possible vehicle routes, which one permits the driver to deliver all parcels the fastest?” Another is asked in telecommunications: “given a set number of approved locations for broadcast antennas, which sites should be used to maximize the reach of mobile phone signal?”

Lastly, and directly related to this post, a financial investor asks: “Given a list of stocks and a budget for how many different stocks can be bought, which assignment maximizes the amount of cash accumulated over time with the minimal amount of risk?”.



Appendix / Page Break

Subheading

Thank You



covalent.xyz



[agnostiqHQ/covalent](https://github.com/agnostiqHQ/covalent)



[@covalentxyz](https://twitter.com/covalentxyz)



Learn more



agnostiq.ai



agnostiqHQ



@agnosticHQ

Manage, deploy & scale workloads across the worlds most advanced computing hardware.

Workflows are composed of python decorators that create what we call lattices and electrons. Electrons are workflow components and lattices are groups of electrons.

