Large-scale Hybrid Quantum Workflows with PennyLane

XANADU

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PENNYLANE

Pennylane is *the* leading open-source library for researchers
to build state-of-the-art hybrid & device agnostic quantum algorithms.

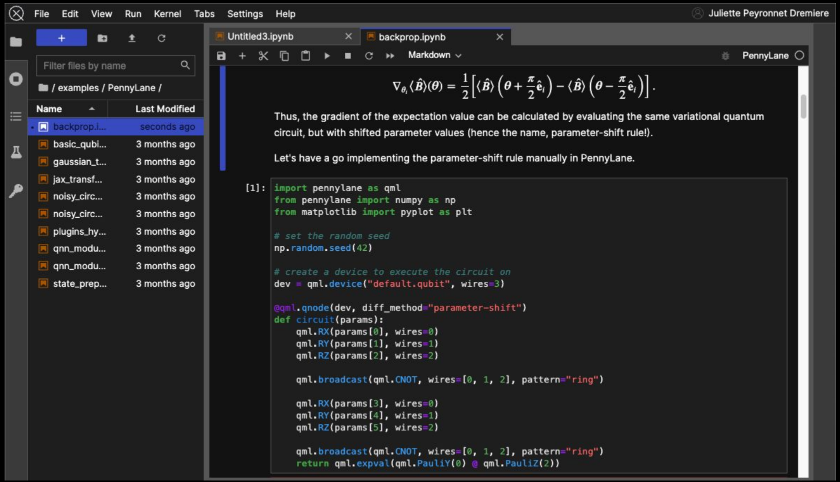
```python
dev = qml.device("qiskit.ibmq", wires=2)

@qml.qnode(dev, diff_method="parameter-shift")
def fn1(x):
  qml.RX(x, wires=0)
  qml.CNOT(wires=[0, 1])
  return qml.expval(qml.PauliZ(0))

dev = qml.device("default.qubit.tf", wires=2)

@qml.qnode(dev, diff_method="backprop")
def fn2(x):
  qml.RY(x, wires=1)
  qml.CZ(wires=[0, 1])
  return qml.probs(wires=0)

def cost(x):
  return fn1(x)**2 - tf.reduce_sum(tf.sin(fn2(x)))
```



GitHub:PennyLaneAI/pennylane

We work with a lot of people, in a lot of places...

Hardware

Fabrication partners and component suppliers.

Software

Channel and software partners for Xanadu Cloud and PennyLane.

Applications

Quantum application and algorithm development.

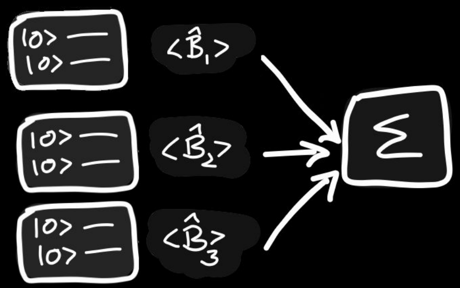
…to support Quantum programming on any platform

Integrated Photonics	Trapped Ions	ML Tools
XANADU	QUANTINUUM AQT IONQ	PyTorch NumPy TensorFlow JAX

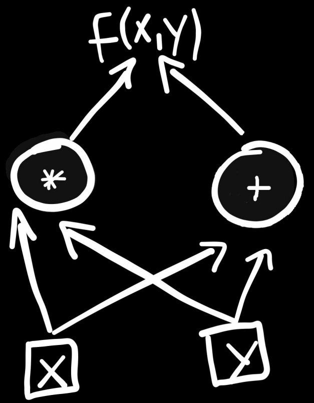
Superconducting Qubits	Quantum Simulators	Platforms
IBM rigetti	Google Microsoft	aws HPC

…with compositions of hybrid Quantum & Classical Computations…

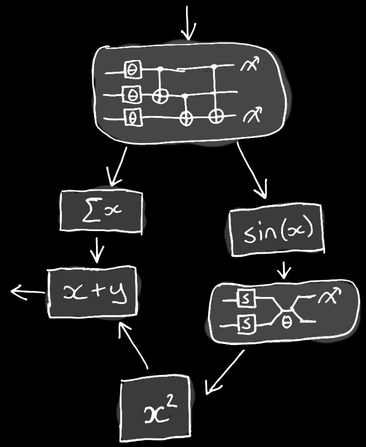
Support for arbitrary hybrid quantum-classical models; every PennyLane computation is end-to-end differentiable



Trainable circuit



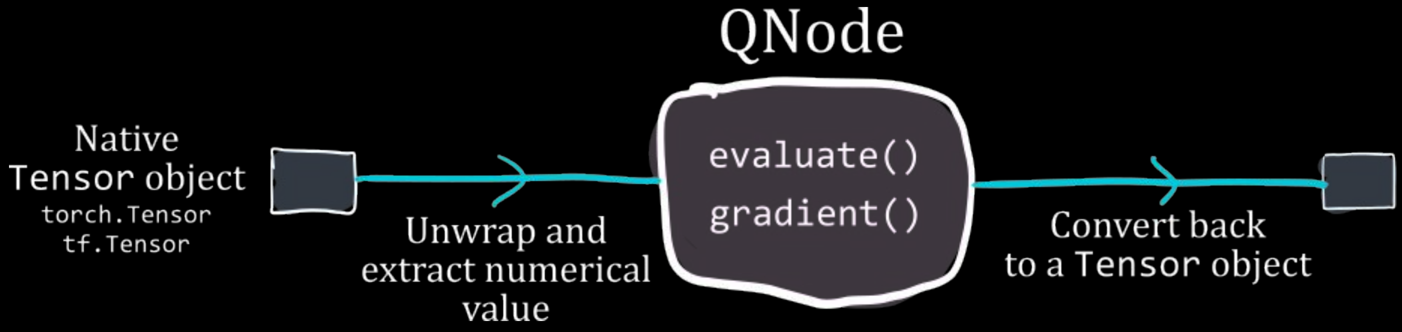
Trainable classical model



Rich, end-to-end trainable hybrid model

…with help from Quantum Nodes (QNode)

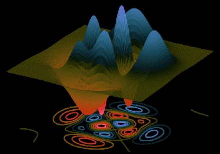
QNodes interface between quantum computers and classical scientific libraries



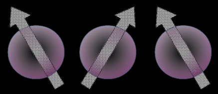
NumPy PyTorch TensorFlow

Plenty of examples to go around

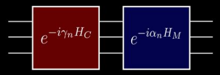
State preparation with pytorch



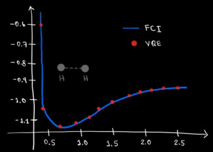
3-qubit ising model



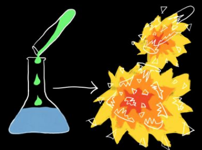
QAOA



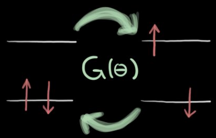
VQE



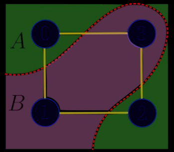
Modeling chemical reactions



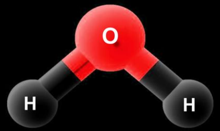
Givens rotations for quantum chemistry



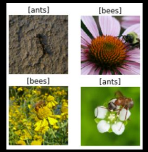
QAOA for MaxCut



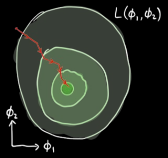
Building molecular hamiltonians



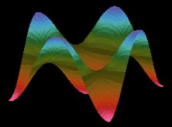
Quantum transfer learning



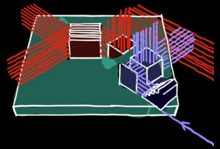
Quantum natural gradient



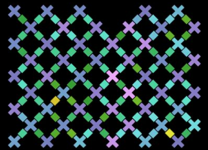
Barren plateaus in quantum neural networks



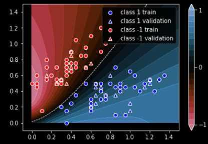
Quantum advantage with GBS



Beyond classical computing with qsim



Variational classifier



See more at pennylane.ai/qml

PennyLane on HPC platforms

Focus on best tools for the task at hand

PENNYLANE DISTRIBUTED

INDUSTRY STANDARD FOR HPC TOOLING

OpenMP

ML FRAMEWORKS INTEGRATION

PyTorch

TensorFlow

DISTRIBUTED WORKLOADS

RAY

DASK

PennyLane-Lightning: run performant simulations on all machines, great (HPC) and small (laptop)

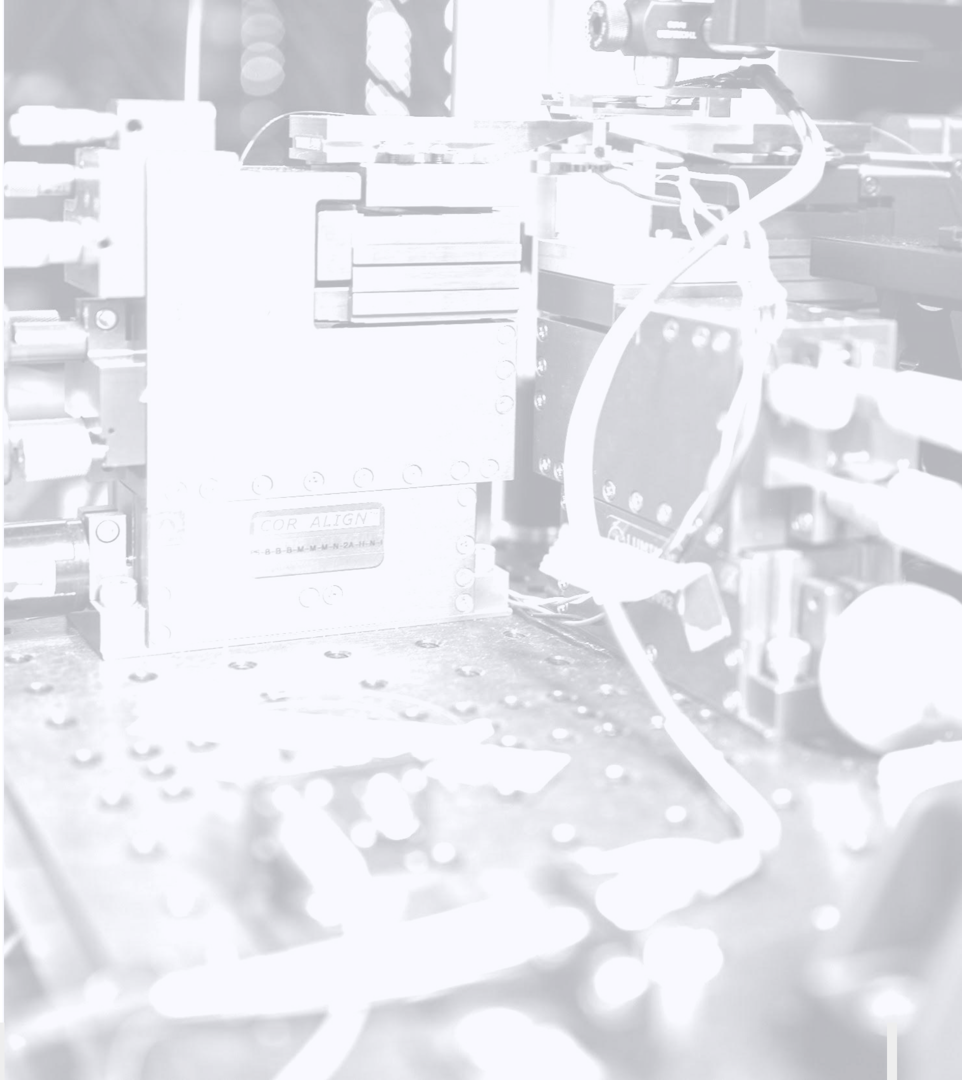
Device	Platforms	Unique feature
`lightning.qubit`	• **Windows**: x86_64 • **MacOS**: x86_64, ARM • **Linux**: x86_64, ARM, PPC, etc. `pip install pennylane-lightning`	• Modern C++20 codebase — compiles & runs everywhere a supported compiler does • Batching of observable gradients (OpenMP) • Automatically dispatched SIMD gate kernels • Comes by default with `pip install pennylane`

`lightning.gpu`	• **Linux w/ CUDA**: x86_64, ARM*, PPC*
	`pip install pennylane-lightning[gpu]`
	`pip install cuquantum`
		• Optimal NVIDIA GPU performance through cuQuantum
		• Native GPU support for adjoint backpropagation
		• Batching of observable gradients over multiple GPUs

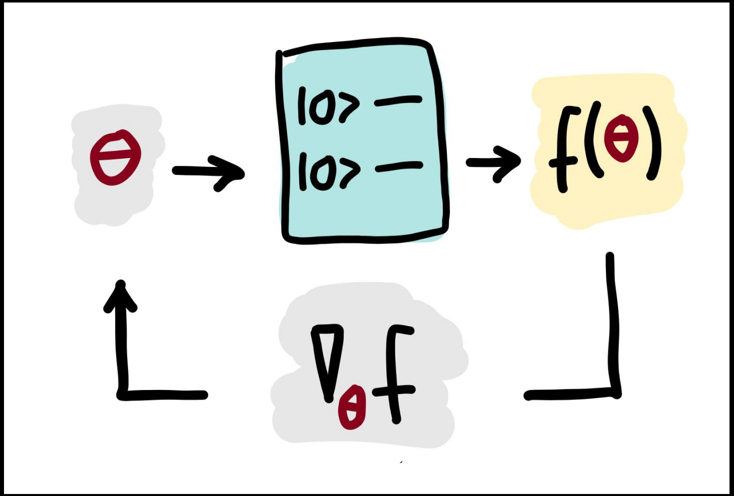
NEW! `lightning.kokkos`	• **Mac & Linux**: All CPUs & GPUs supported by Kokkos-Core (Intel, NVIDIA, AMD, etc) • `PennyLaneAI/pennylane-lightning-kokkos`	• Multithreaded gate applications (OpenMP, C++ threads) • Accelerator device execution models natively supported (CUDA, HIP/ROCm, SYCL)

Goal: Build tooling that is useful

Variational quantum optimization problems (with circuit cutting)



Variational algorithms & gradients



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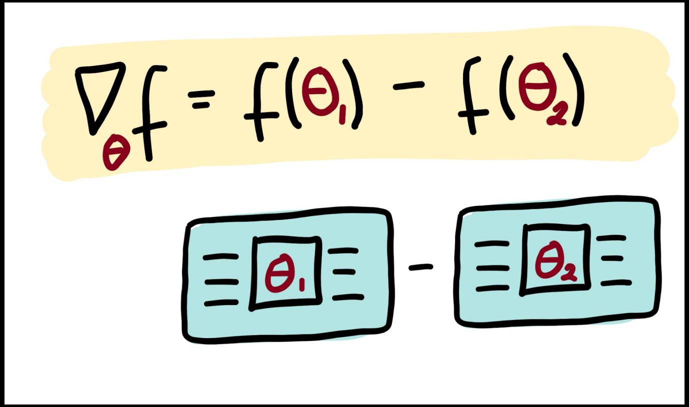
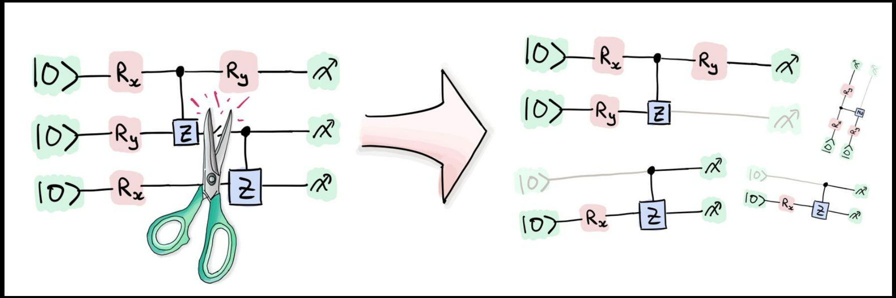
Quantum circuits natively differentiable

Both **finite difference** and
parameter-shift methods have the form:



For N parameters, number
of evaluations is **O(2N)**

Detour into Circuit cutting: A Tensor Network is a Quantum Circuit is a Tensor Netw…



Cut qubit indices & Cut gate tensors

- Break a large circuit into multiple smaller circuits
- Circuits must be “stitched” back together classically (sums/contractions)
- Multiple smaller circuits can be run independently of one another

Q: Can we farm these circuits out to some combination of CPUs/GPUs/QPUs?

A: Yes! But first, let’s see an example.

Quantum programs can be cut into fragments and executed with very small changes to code

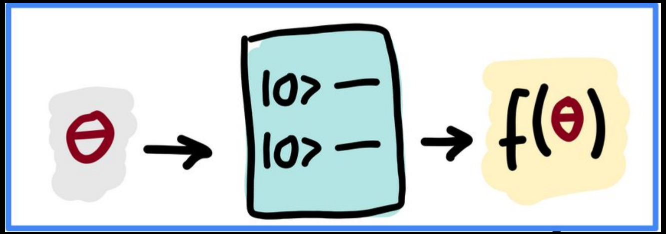
```python
import pennylane as qml
from pennylane import numpy as np

#Two qubit device
dev = qml.device("lightning.qubit", wires=2)

@qml.cut_circuit              # Enable circuit cutting
@qml.qnode(dev)
def circuit(param):           # Build 3-qubit circuit
    qml.RX(param, wires=0)
    qml.RY(0.9, wires=1)
    qml.RX(param, wires=2)
    qml.CZ(wires=[0,1])
    qml.RY(-0.4, wires=0)
    qml.WireCut(wires=1)      # Add wire-cut
    qml.CZ(wires=[1,2])

    return qml.expval(qml.PauliZ(0) @ qml.PauliZ(1) @ qml.PauliZ(2))
```

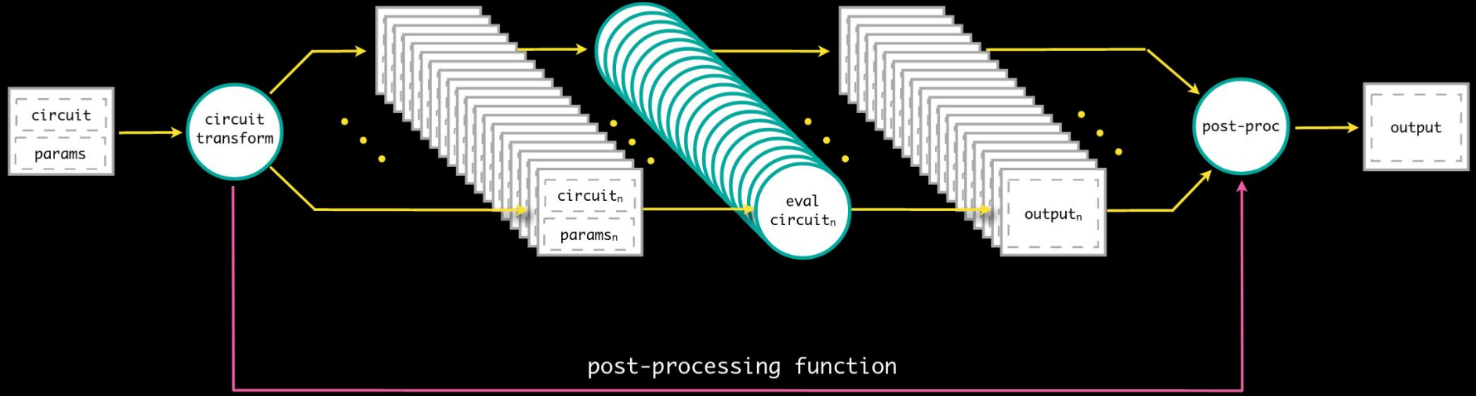
- Create a two qubit device
- Enable the circuit cutting functionality
- Build a 3 qubit circuit
- Specify wire-cuts

Circuit cutting and stitching is automated for user

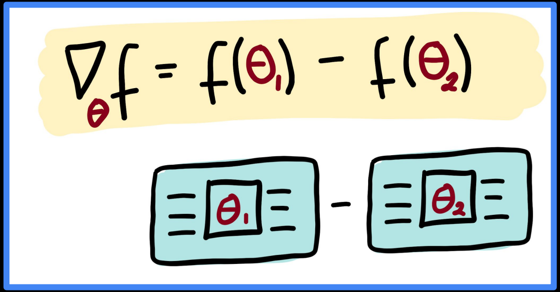
```python
>>> my_param = np.array(0.1523, requires_grad=True)
>>> circuit(my_param), qml.grad(circuit)(my_param)
(0.5593628104920161, -0.17171160308785013)
```

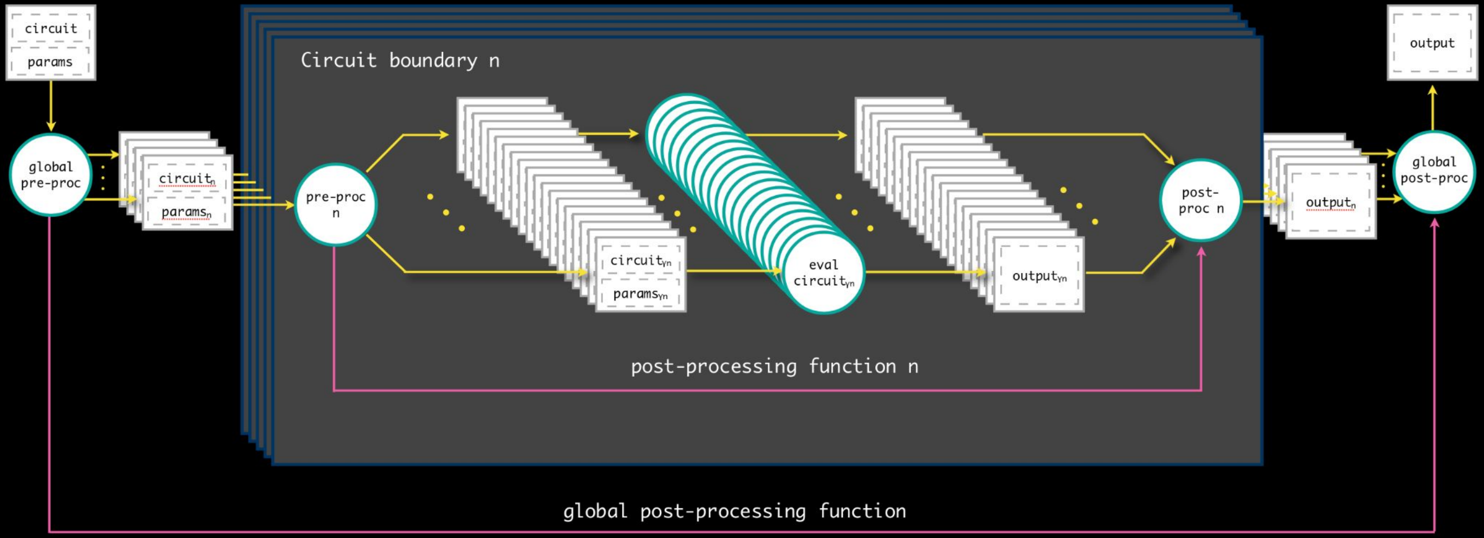
Circuit execution model



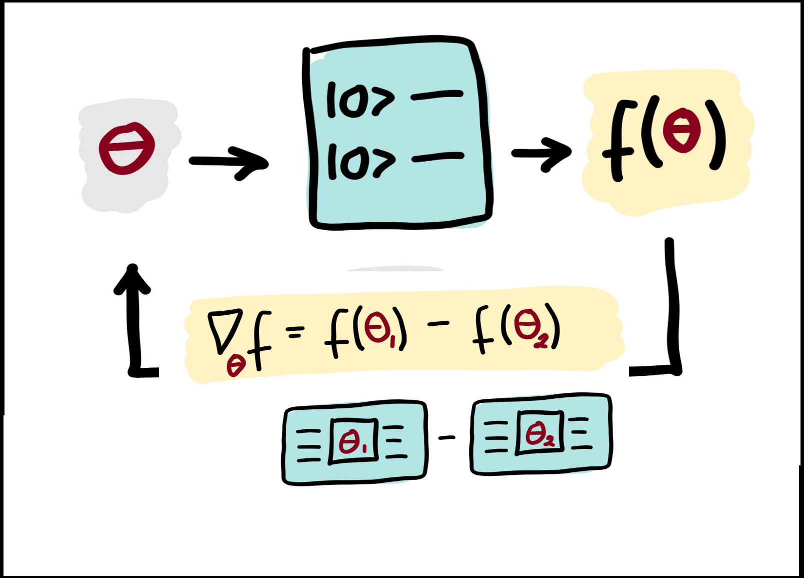


Circuit execution model





Quantum parameter optimization for QAOA



1. Calculate the variational energy for a 129 qubit QAOA clustered graph problem

2. Variational parameter optimization of a 62 qubit QAOA problem

- **For analytical results, see paper**

arxiv:2207.14734

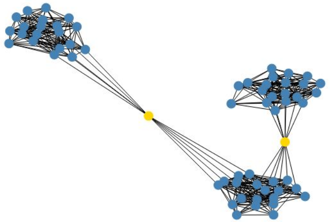
Fast quantum circuit cutting with randomized measurements

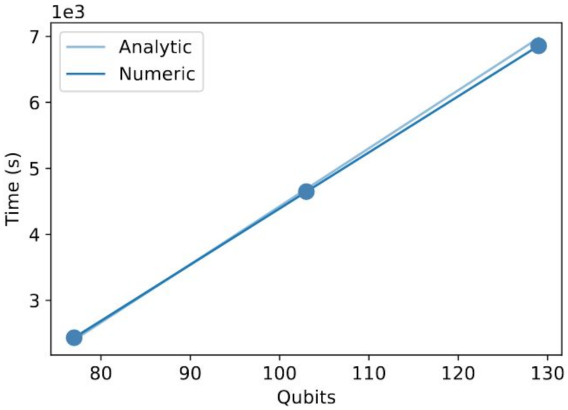
Angus Lowe,[1] Matija Medvidović,[1,2,3] Anthony Hayes,[1] Lee J. O'Riordan,[1] Thomas R. Bromley,[1] Juan Miguel Arrazola,[1] and Nathan Killoran[1]

[1] *Xanadu, Toronto, ON, M5G 2C8, Canada*
[2] *Center for Computational Quantum Physics, Flatiron Institute, 162 5th Avenue, New York 10010, USA*
[3] *Department of Physics, Columbia University, New York 10027, USA*

Numerical results

1. Variational energy calculation upto 129 qubits

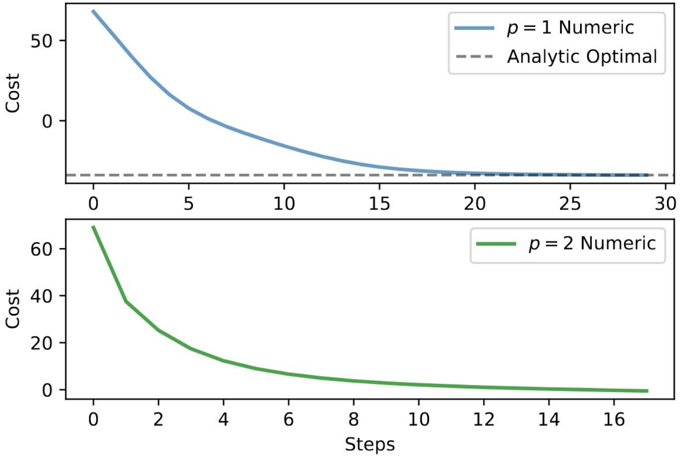




2 QAOA circuit layers (p=2)
25 nodes per cluster (n=25)
1 node per inter-cluster connection (k=1)

Clusters varied to increase qubit requirements (r)

2. Parameter optimization on 62 qubits



(2.a) p=1,n=20,k=1,r=3: ~0.5 hr @ 2 GPU nodes

(2.b) p=2,n=20,k=1,r=3: ~12 hr @ 10 GPU nodes

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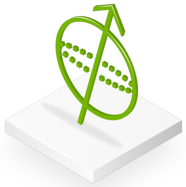
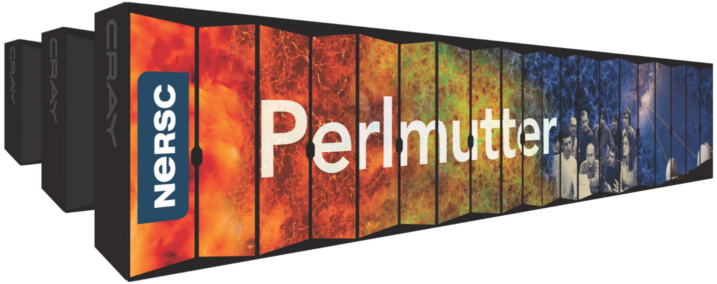
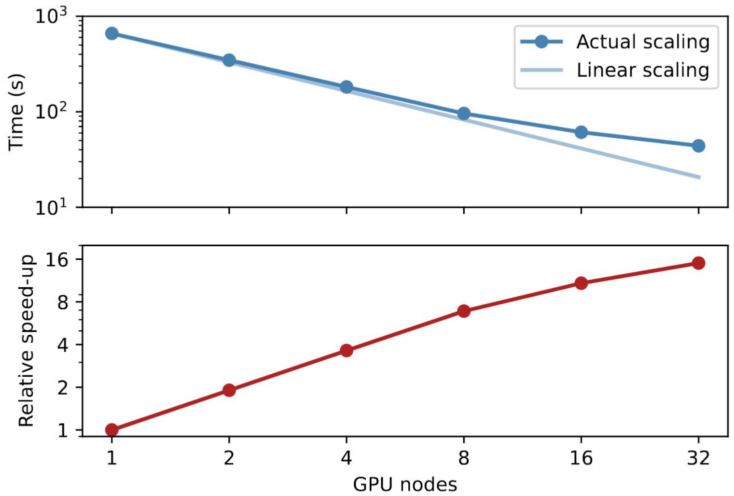




Scaling results for for a 79 qubit problem



p=1,n=25,k=2,r=3 vs GPU resources

GitHub:XanaduAI/randomized-measurements-circuit-cutting

Thank you!

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xanadu.ai // **pennylane.ai**

arxiv:2207.14734

GitHub:XanaduAI/randomized-measurements-circuit-cutting