Quantum Software/Simulation/Tools

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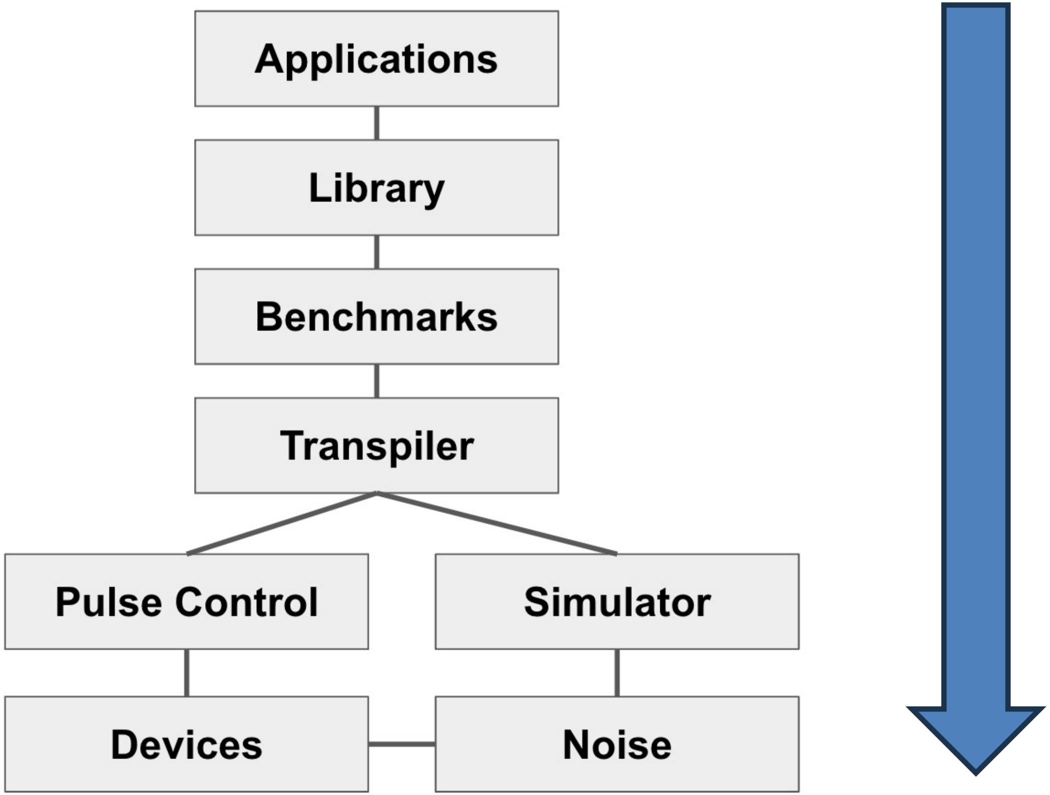
Quantum Software Stack



Applications

Library

Benchmarks

Transpiler

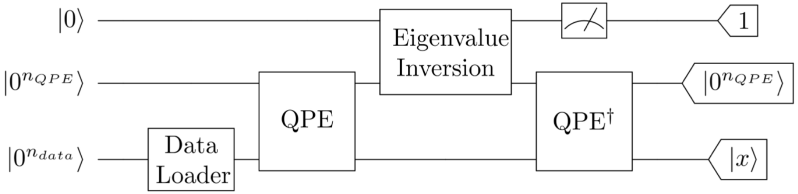
Pulse Control

Simulator

Devices

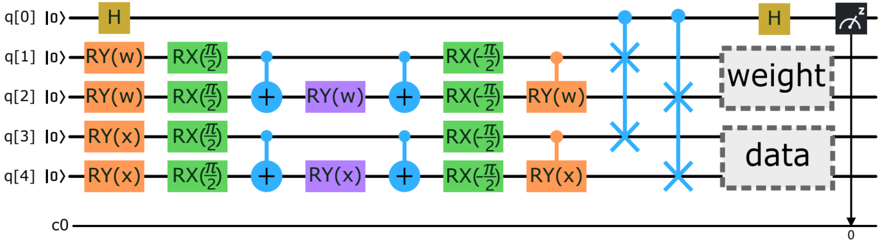
Noise

Application-1: Power Grid

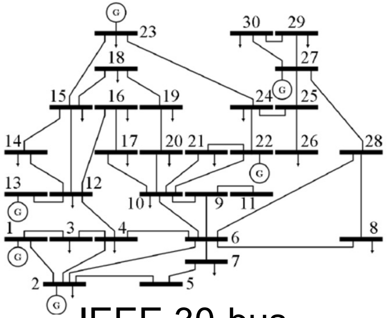


HHL components

	14-bus	30-bus	30-bus*
Matrix Size	13×13	29×29	29×29
Condition Number	119.2	492.5	109.3
n_{total} and $(n_{\text{data}}, n_{\text{QPE}})$	13 and (4,8)	16 and (5,10)	15 and (6,8)
Circuit Generation Time	88s	30.5 min	37.5 min
Qiskit Aer Simu. Time	27s	31.3 min	37.5 min
- Error $\|\mathbf{x}_{hhl} - \mathbf{x}_{true}\|_2$	$1.97 \cdot 10^{-3}$	$1.18 \cdot 10^{-3}$	$6.35 \cdot 10^{-4}$
SV-Sim Simu. Time	13s	3.9min	4.7 min
- Error $\|\mathbf{x}_{hhl} - \mathbf{x}_{true}\|_2$	$1.97 \cdot 10^{-3}$	$1.18 \cdot 10^{-3}$	$6.35 \cdot 10^{-4}$



QML circuit example



IEEE 30-bus

Binary classification
Train: 20 cases

- 5-qubit QNN: 72.2%
- 4-layer, 256 neuron: 72.4%

Comparable performance, but 97% less parameters

- Solve large-scale linear systems of equations for power flow analysis
- QML for contingency analysis on predicting bus voltage violation

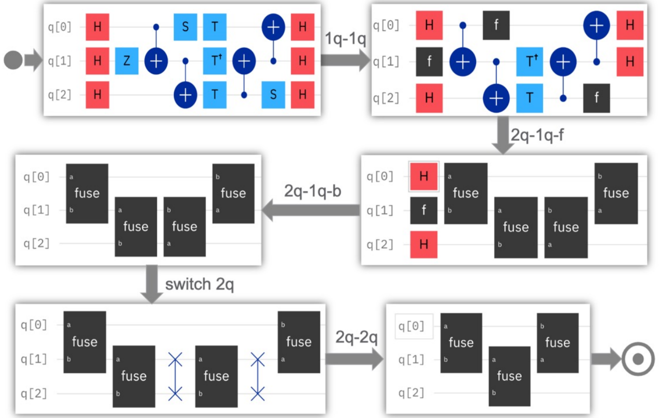
[1] Muqing Zheng, Yousu Chen, Xiu Yang and Ang Li. "Early Exploration of a Flexible Framework for Efficient Quantum Linear Solvers in Power Systems." arXiv:2402.08136, IEEE Power and Energy Society General Meeting, 2024.

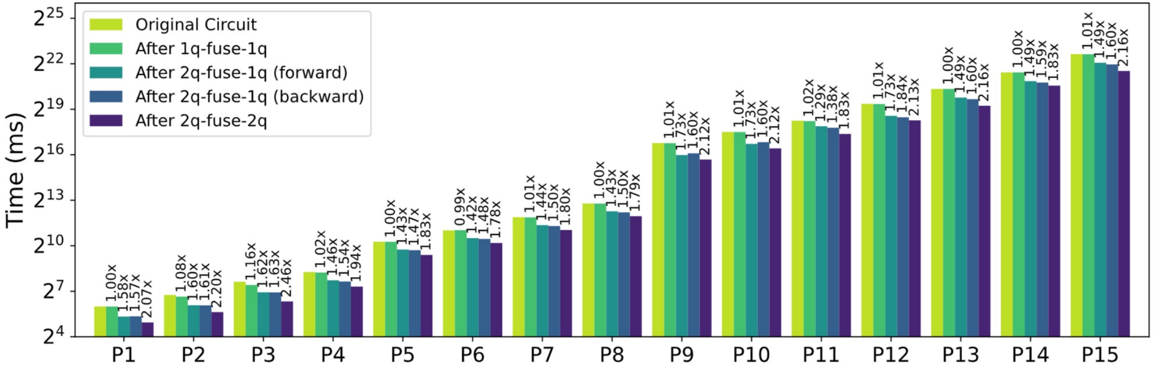
[2] Yousu Chen, Zhenyu Huang, Shuangshuang Jin. and Ang Li, 2022. Computing for power system operation and planning: Then, now, and the future. iEnergy, 1(3), pp.315-324.

Application-2: Low-Energy Nuclear

Shell	N_p	N_n	N_q^{JW}	N_{Pauli}^{JW}	N_q^{SM}	N_{Pauli}^{SM}
p	1	2	12	975	5	528
p	2	2	12	975	6	2,072
p	1	3	12	975	5	488
p	2	3	12	975	6	2,080
p	3	3	12	975	7	7,936
sd	1	2	24	12,869	7	8,252
sd	1	3	24	12,869	9	131,321
sd	2	2	24	12,869	10	523,720

Problem	Nucleus	Trotter	Success Rate	E_{exact} (MeV)	E_{sim} (MeV)	Kernel Time	Gates	2-Qubit Gates
P1	^{6}He	8	26.90%	-3.910	-2.645	30.8ms	11,939	7,088
P2	^{6}He	14	40.87%	-3.910	-3.362	39.4ms	20,885	12,404
P3	^{6}He	26	40.35%	-3.910	-3.808	80.4ms	38,777	23,036
P4	^{6}He	47	37.33%	-3.910	-3.902	158.4ms	70,088	41,642
P5	^{20}O	14	27.25%	-35.267	-34.898	672.8ms	210,457	126,980
P6	^{20}O	24	38.17%	-35.267	-35.149	1.16s	360,767	217,680
P7	^{20}O	44	41.69%	-35.267	-35.228	2.10s	661,387	399,080
P8	^{20}O	83	42.53%	-35.267	-35.255	3.95s	1,247,596	752,810
P9	^{44}Ca	18	3.77%	-5.006	-4.334	52.62s	1,970,931	1,208,052
P10	^{44}Ca	30	10.01%	-5.006	-4.536	87.68s	3,284,871	2,013,420
P11	^{44}Ca	58	12.92%	-5.006	-4.853	169.50s	6,350,731	3,892,612
P12	^{44}Ca	108	13.60%	-5.006	-4.917	315.59s	11,825,481	7,248,312
P13	^{44}Ca	214	13.76%	-5.006	-4.939	625.60s	23,431,951	14,362,396
P14	^{44}Ca	528	13.76%	-5.006	-4.944	25.7min	57,813,381	35,436,192
P15	^{44}Ca	1051	13.74%	-5.006	-4.945	56.5min	115,079,266	70,536,814

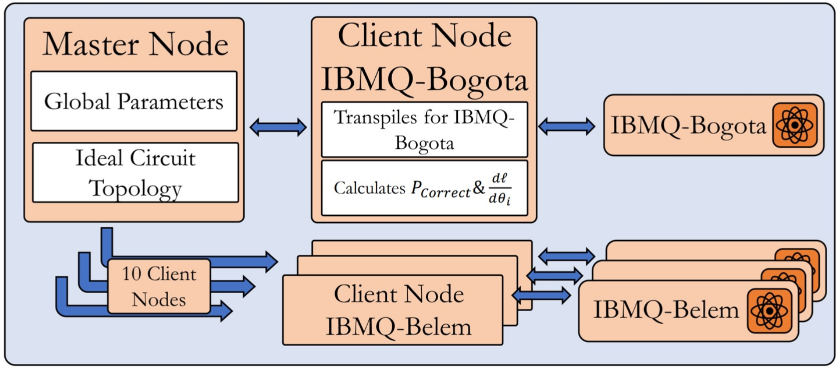




Ang Li, Alessandro Baroni, Ionel Stetcu, and Travis S. Humble. "Deep quantum circuit simulations of low-energy nuclear states." arXiv:2310.17739, The European Physical Journal A. DOI:10.1140/epja/s10050-024-01286-7 (Accepted)

Library: Distributive Variational Quantum Algorithm

- Proposed an ensemble way of building up VQA backends
  - First DVQA training framework for DQC via classical interconnect
  - Using an analytical model for assessing the quality of returned gradients and update asynchronously



Master Node

Global Parameters

Ideal Circuit Topology

Client Node IBMQ-Bogota

Transpiles for IBMQ-Bogota

Calculates $P_{Correct}$ & $\frac{d\ell}{d\theta_i}$

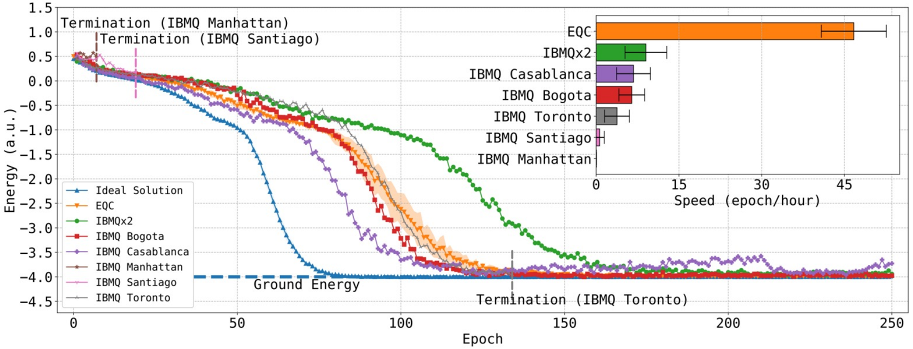
IBMQ-Bogota

10 Client Nodes

Client Node IBMQ-Belem

IBMQ-Belem

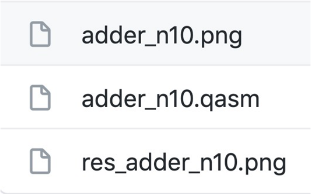
- Evaluation on 10 IBMQ devices
  - Average 10X on VQE/QAOA training
  - Improved fidelity due to averaging-out machine-specific bias



[1] S. Stein, N. Wiebe, Y. Ding, P. Bo, K. Kowalski, N. Baker, J. Ang, and A. Li. "EQC: ensembled quantum computing for variational quantum algorithms." In *ACM/IEEE International Symposium on Computer Architecture (ISCA)*, 2022, DOI: 10.1145/3470496.3527434.

Benchmark: QASMBench

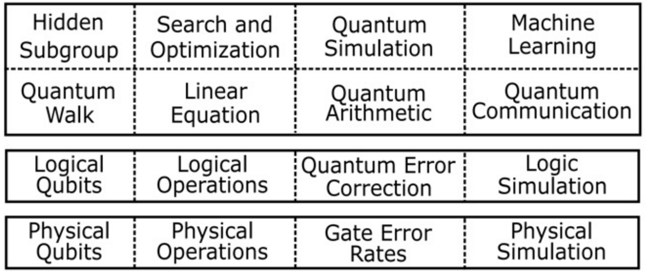
- Benchmark coverage
  - Qubits from 2 to 1000
  - Gates from 4 to 2.3M
  - ~80 circuits covering different domains
- Each benchmark



adder_n10.png <= Circuit visualization
adder_n10.qasm <= OpenQASM code
res_adder_n10.png <= IBM-Q result histogram

- Evaluated on IBMQ and IonQ
- Propose circuit metrics

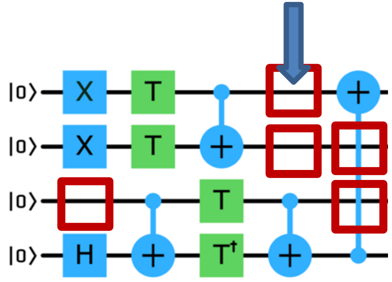
$$\text{Gate Density} = \frac{G_{\text{1-qubit}} + 2 \times G_{\text{2-qubit}}}{\text{Circuit Depth} \times \text{Circuit Width}}$$



Hidden Subgroup	Search and Optimization	Quantum Simulation	Machine Learning
Quantum Walk	Linear Equation	Quantum Arithmetic	Quantum Communication
Logical Qubits	Logical Operations	Quantum Error Correction	Logic Simulation
Physical Qubits	Physical Operations	Gate Error Rates	Physical Simulation

A. Montanaro "Quantum algorithms: an overview." npj Quantum, 2016

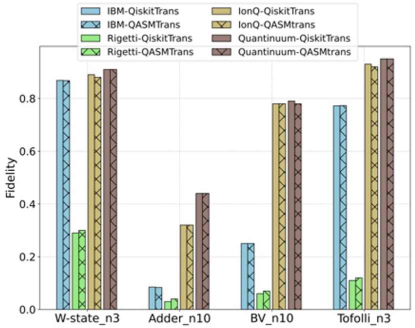
ID Gate



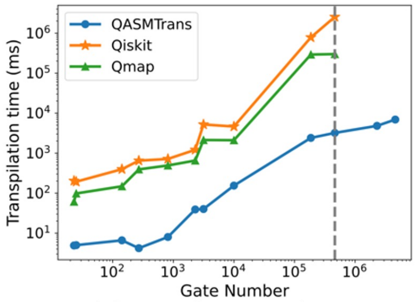
Gate Density =15/20

[1] A. Li, S. Stein, S. Krishnamoorthy, and J. Ang. "QASMBench: A low-level QASM benchmark suite for NISQ evaluation and simulation." ACM Transactions on Quantum Computing, 2022, DOI: 10.1145/3550488

Transpiler: QASMTrans



(A) Fidelity consistency with Qiskit



(B) Transpile time with gates

(A) QASMTrans obtains comparable fidelity for the transpiled circuit with respect to Qiskit on four real NISQ devices: IBM-Brisbane, Rigetti-AspenM2, IonQ-Aria1 and Quantinuum-H1-1. (B) Transpilation time with respect to gates of the input circuits. The last two cannot be transpiled in 1 hour by Qiskit and Qmap but 31s and 69s by QASMTrans.

Fei Hua, Meng Wang, Gushu Li, Bo Peng, Chenxu Liu, Muqing Zheng, Samuel Stein, Yufei Ding, Eddy Z. Zhang, Travis S. Humble, Ang Li. "QASMTrans: A QASM based Quantum Transpiler Framework for NISQ Devices." arXiv preprint arXiv:2308.07581 (2023), Accepted at Fourth International Workshop on Quantum Computing Software (with SC23). Full paper in-development.

* Code is released at https://github.com/pnnl/qasmtrans

- IPID 32821-E, Export Control: ERA99, PNNL-SA-188499
- Software DOI: 10.11578/dc.20230814.4

Achievement

Developed a high-performance C++ quantum transpiler that can demonstrate a 10-369x speedup over Qiskit.

Significance and Impact

Significantly accelerated the compiling speed of deep circuits, allowing the exploration of much larger design space, more comprehensive compiler optimizations, and practical development, providing a seed code for transpiler research.

Details

- QASMTrans implements and improves state-of-the-art decomposition, mapping, and routing approaches over currently-available quantum transpilers.
- The framework features a pure C++ design without external library dependencies, allowing it to achieve high performance even on an ARM8 processor, permitting potential deployment to the FPGA of a quantum control plane.
- Evaluated fidelity on IBMQ, Quantinuum, IonQ and Rigetti. Evaluated transpilation performance on OLCF Frontier, Summit, NERSC Perlmutter, ALCF Theta, Apple M2 and Jetson TX2.

NWQ-Sim Framework

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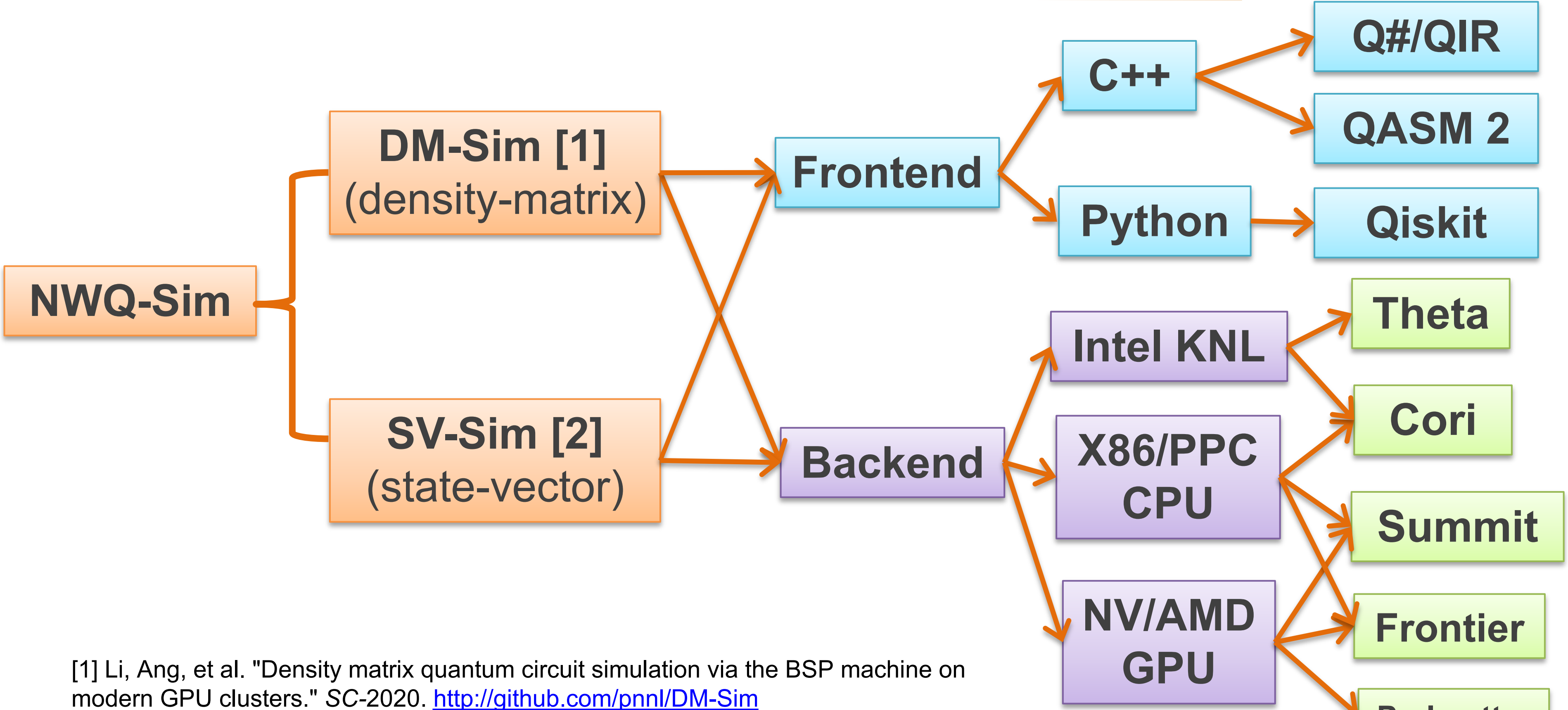


NWQ-Sim

DM-Sim [1]
(density-matrix)

SV-Sim [2]
(state-vector)

Frontend

Backend

C++

Python

Q#/QIR

QASM 2

Qiskit

Intel KNL

X86/PPC CPU

NV/AMD GPU

Theta

Cori

Summit

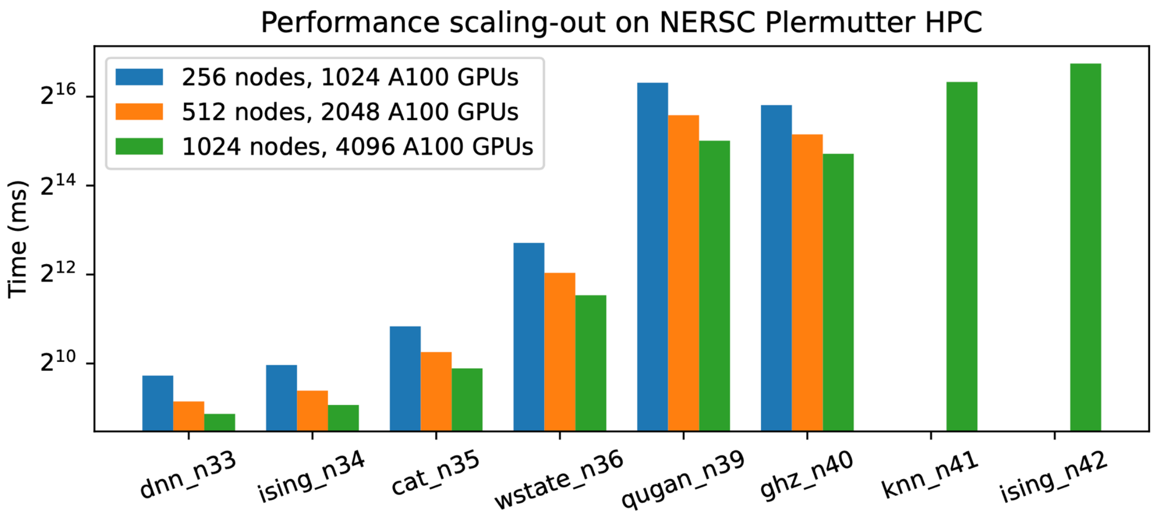
Frontier

Perlmutter

[1] Li, Ang, et al. "Density matrix quantum circuit simulation via the BSP machine on modern GPU clusters." *SC*-2020. http://github.com/pnnl/DM-Sim
[2] Li, Ang, et al. “SV-Sim: Scalable PGAS-based State Vector Simulation of Quantum Circuits”, *SC*-2021. http://github.com/pnnl/SV-Sim

Supported by DOE, Quantum Science Center (QSC)

SV-Sim strong-scaling on Perlmutter

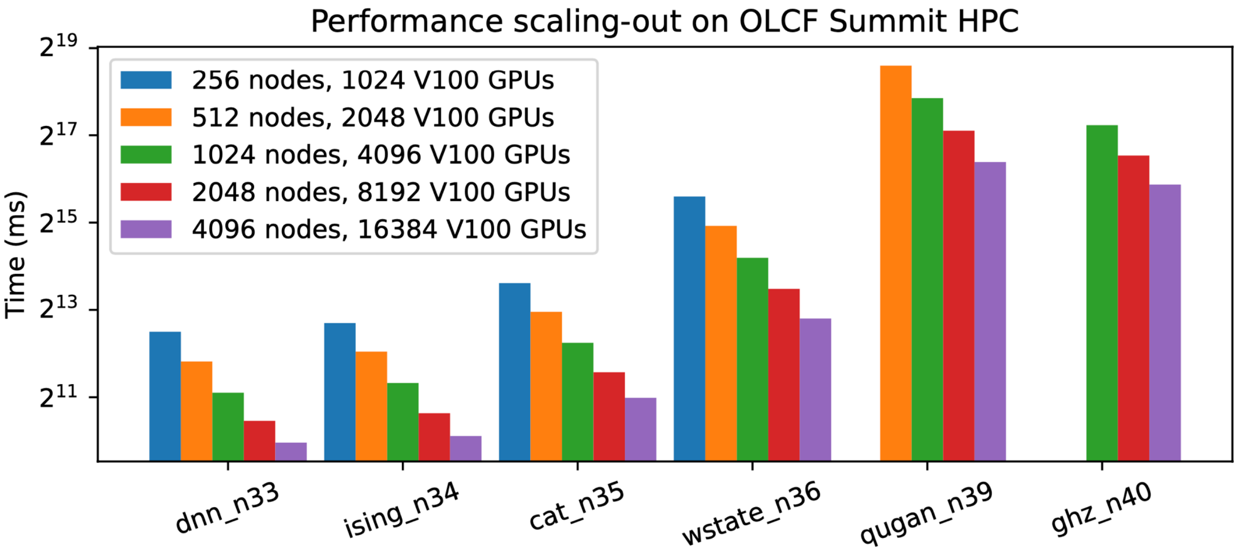


Circuit	Qubits	Gates	Sim_gates	Mem (MB)
dnn_n33	33	489	143	262144
ising_n34	34	369	36	524288
cat_n35	35	36	35	1048576
wstate_n36	36	142	71	2097152
qugan_n39	39	652	187	16777216
ghz_n40	40	41	40	33554432
knn_n41	41	383	123	67108864
ising_n42	42	457	44	134217728

Application	GPU	Gates	Time (ms)	Gates/s
knn_n41	4096	383	82437	4.6
ising_n42	4096	457	109848	4.2

- Performance strong-scaling on Perlmutter A100 GPUs
- 42-qubit state-vector simulation entirely on 4096 GPUs
- On-average 4.2 gates/s at 42-qubit scale (32GB/GPU)

SV-Sim strong-scaling on Summit



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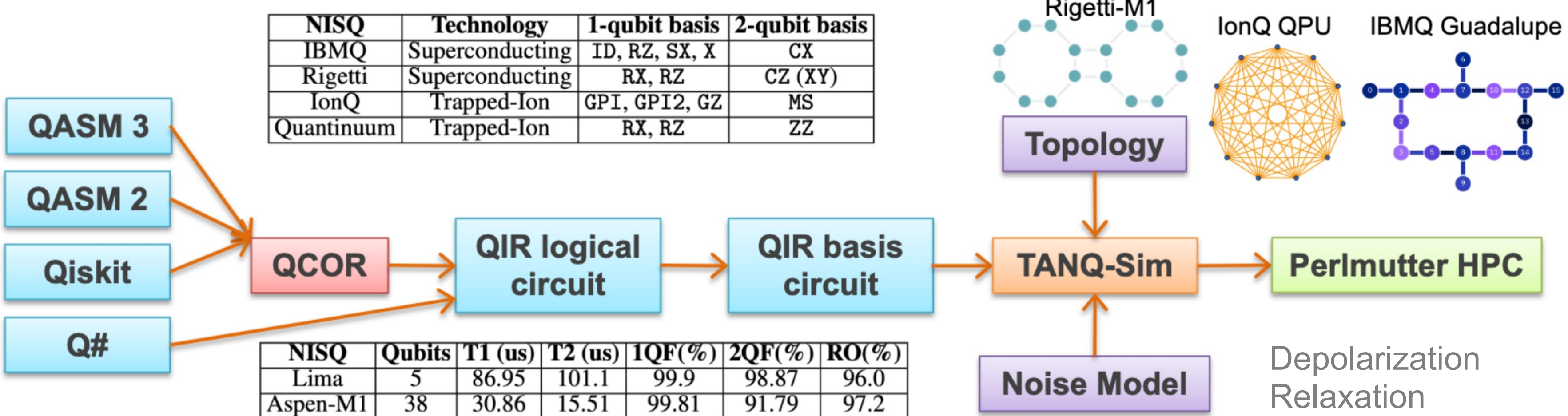
knn_n41	41	383	123	67108864
ising_n42	42	457	44	134217728

- Performance strong-scaling on Summit V100 GPUs
- 40-qubit state-vector simulation over 16,384 GPUs (8GB/GPU)

Density Matrix Simulation



QASM 3

QASM 2

Qiskit

Q#

QCOR

QIR logical circuit

QIR basis circuit

Topology

TANQ-Sim

Noise Model

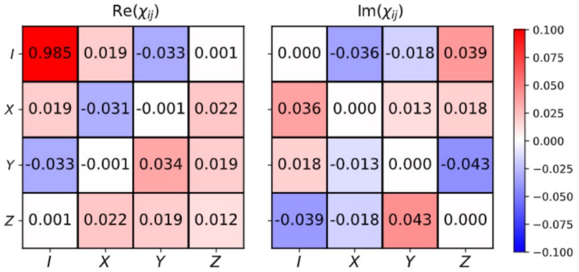
Perlmutter HPC

NISQ	Technology	1-qubit basis	2-qubit basis
IBMQ	Superconducting	ID, RZ, SX, X	CX
Rigetti	Superconducting	RX, RZ	CZ (XY)
IonQ	Trapped-Ion	GPI, GPI2, GZ	MS
Quantinuum	Trapped-Ion	RX, RZ	ZZ

NISQ	Qubits	T1 (us)	T2 (us)	1QF(%)	2QF(%)	RO(%)
Lima	5	86.95	101.1	99.9	98.87	96.0
Aspen-M1	38	30.86	15.51	99.81	91.79	97.2
IonQ QPU	5	1E7	3E6	99.35	96.02	99.3
HQS2	12	3E6	N/A	N/A	99.5	N/A

T1, T2, duration, etc.

Depolarization
Relaxation
SPMA



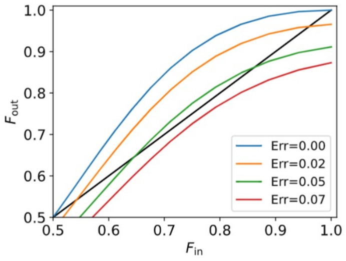
Re(χ_{ij})

	I	X	Y	Z
I	0.985	0.019	-0.033	0.001
X	0.019	-0.031	-0.001	0.022
Y	-0.033	-0.001	0.034	0.019
Z	0.001	0.022	0.019	0.012

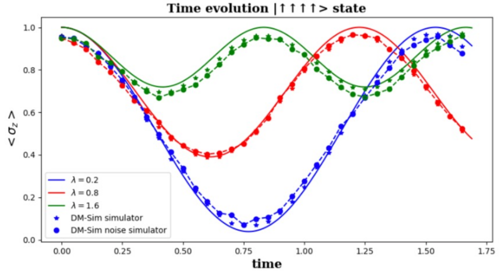
Im(χ_{ij})

	I	X	Y	Z
I	0.000	-0.036	-0.018	0.039
X	0.036	0.000	0.013	0.018
Y	0.018	-0.013	0.000	-0.043
Z	-0.039	-0.018	0.043	0.000

Teleportation



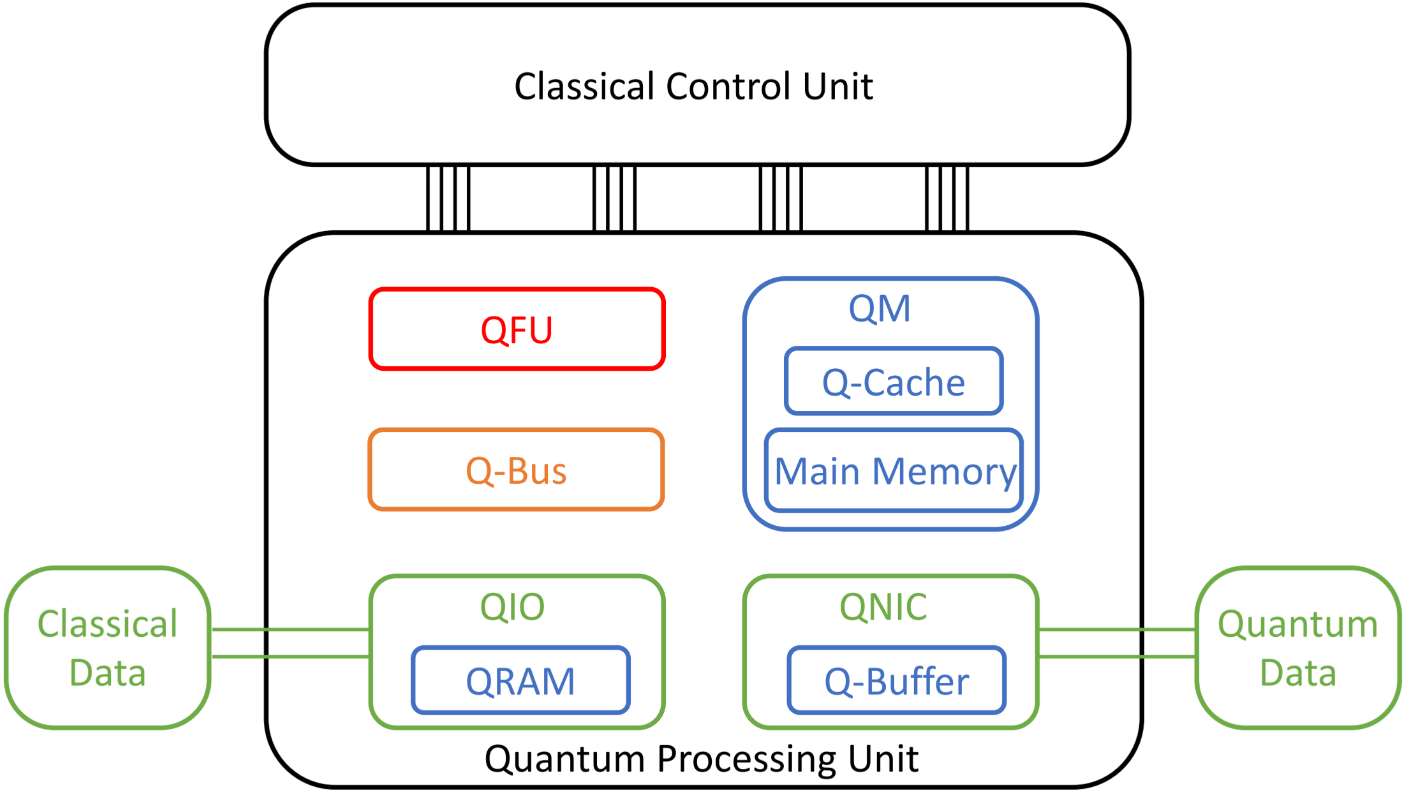
Distillation



Ising Simulation

[1] A. Li et al, "TANQ-Sim: Tensorcore Accelerated Noisy Quantum System Simulation via QIR on Perlmutter HPC", arXiv:2404.13184

Moving Forward..



[1] Liu, Chenxu, Meng Wang, Samuel A. Stein, Yufei Ding, and Ang Li. "Quantum Memory: A Missing Piece in Quantum Computing Units." arXiv preprint arXiv:2309.14432 (2023).

Acknowledgement

- This work is supported by DOE Office of Science, National Quantum Information Science Research Centers, Co-design Center for Quantum Advantage (C2QA) under contract number DE-SC0012704.
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