Knowledge Compilation-Based Exact Inference for Quantum Simulation

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Resource estimation for quantum simulation

Why is simulation important?

- "Developing good classical simulations (or even attempting to and failing) would also help clarify the quantum/classical boundary."
—Aram Harrow

- Development and debugging of quantum algorithm implementations

How do we build a quantum simulator?

Be very smart and write a lot of code:

- Clever circuit minimizations (Cirq optimizations, Qiskit transpilation…)
- Massive parallelism (QuEST, efforts by IBM, Google, Alibaba…)
- Compression (Wu et al., Supercomputing 2019, BDD-based methods)
- Emulation (ProjectQ)
- Stabilizer formalism (CHP by Aaronson)

Borrow from existing classical techniques…

Outline: Borrowing classical probabilistic inference for quantum simulation

- Connection between quantum circuits and Bayesian networks
- Our toolchain for quantum simulation:
  exact Bayesian network inference based on knowledge compilation
- Evaluation of features offered by this approach:
  structure extraction & more efficient repeated simulation

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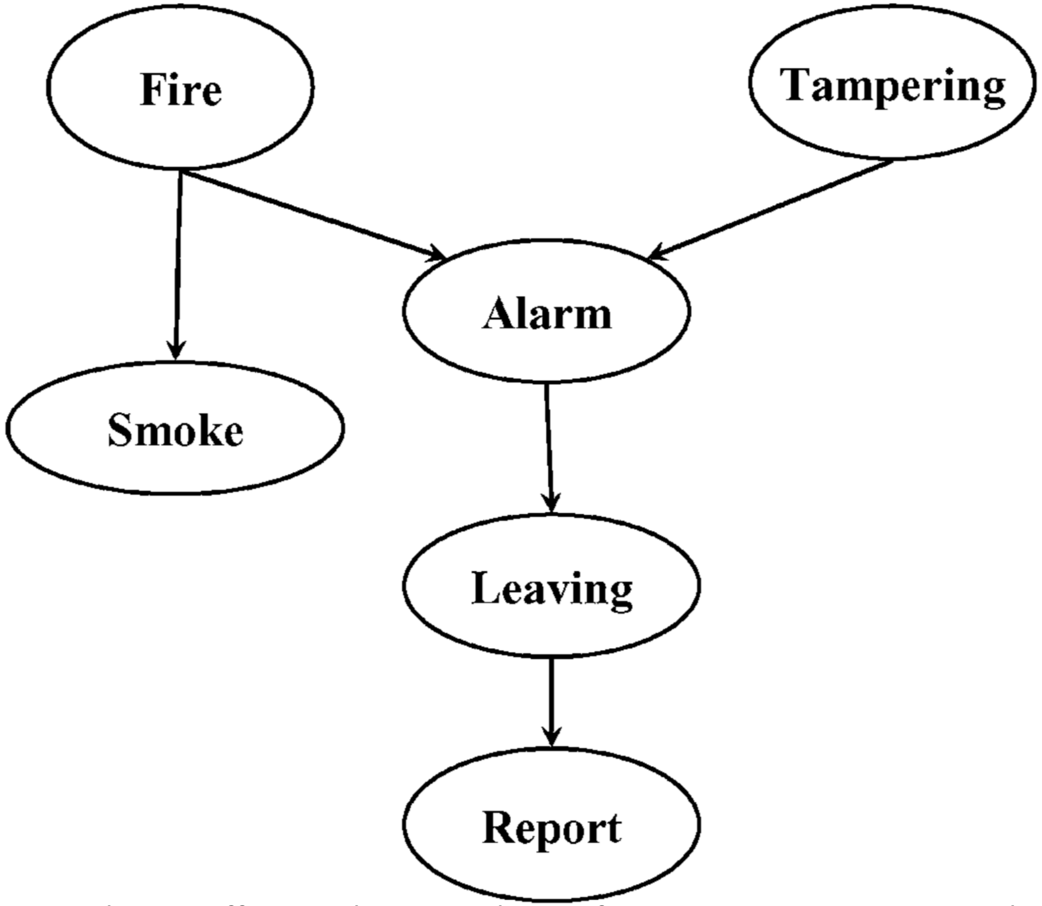
Probabilistic graphical models and an example

Bayesian networks

- AKA directed graphical models, belief networks

Markov networks

- AKA undirected graphical models, Markov random fields



Darwiche, A Differential Approach to Inference in Bayesian Networks

Theory: connection between quantum computing and probabilistic inference

	Quantum	Probabilistic
Key analogies	program simulation	inference
	qubits	random variables
	amplitudes	probabilities
	operator unitary matrices	conditional probability tables
	superposition states	probability distributions
	entangled qubits	dependent random variables
	measurement	sampling & conditioning
Key distinctions	amplitudes are complex-valued	probabilities between 0 and 1
	squares of amplitudes sum to 1	probabilities sum to 1
	interference (canceling of amplitudes) possible	interference impossible

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Quantum / probabilistic: separated by Gottesman-Knill theorem, ideas can cross-pollinate

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Our toolchain for quantum simulation via knowledge compilation exact inference

- Quantum circuit (QASM) to complex-valued Bayesian network
- Bayesian network to conjunctive normal form (CNF)
- CNF to arithmetic circuit (AC)
- Exact inference on AC to obtain quantum simulation

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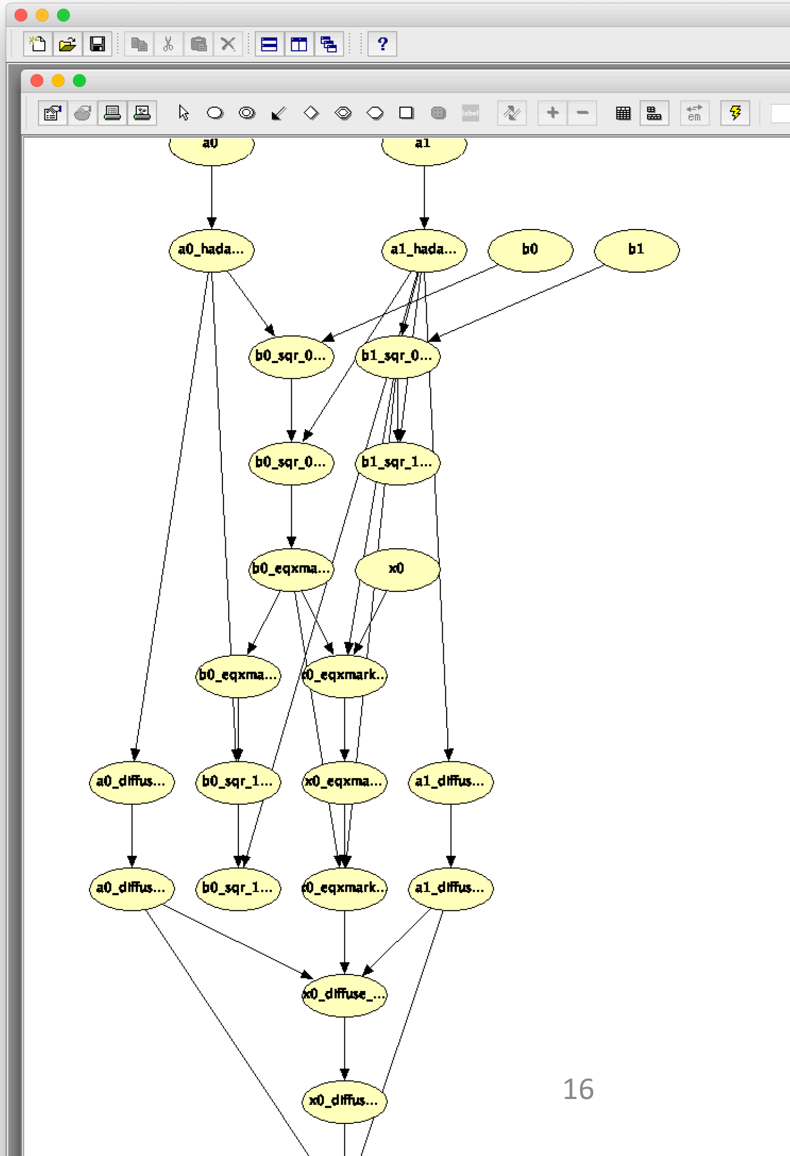
Quantum circuit (QASM) to complex-valued Bayesian network

Quantum circuit DAG
→ Bayesian network topology

Quantum gate unitary matrices
→ conditional probability tables

- Bridge to using classical probabilistic inference
- Similar approach used by Boixo et al.
  for quantum simulation
  (they used Markov undirected networks)



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Bayesian networks to arithmetic circuits

Bayesian network → CNF

- Allows weighted model counting
- Equivalent to Feynman path sum

CNF → arithmetic circuits

- Reduces the circuit size
- ACs are related to BDDs

Many specific techniques, pick one that doesn't assume probabilities sum to 1

- We use UCLA's ACE tool by Chavira & Darwiche

Driven by an underlying solver that needs no special input other than the QASM code

- We use UCLA's C2D tool by Darwiche

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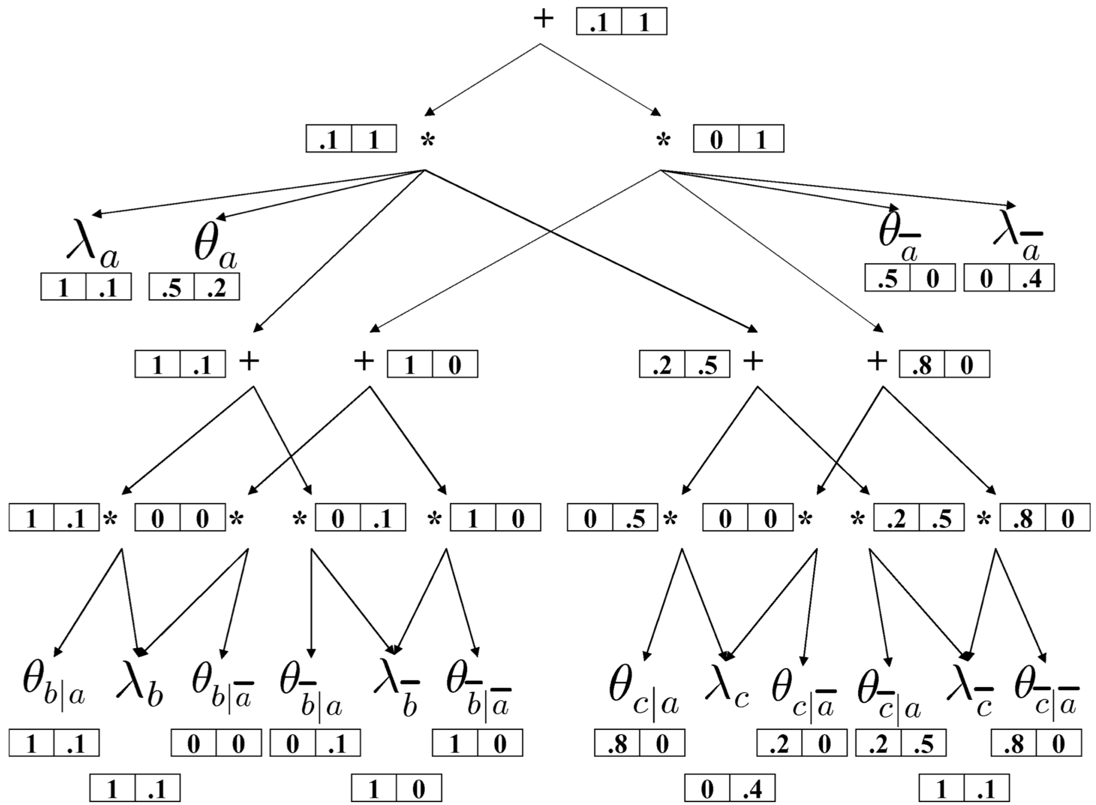
Exact inference on AC to obtain quantum simulation

- Quantum simulation becomes tree traversal on AC

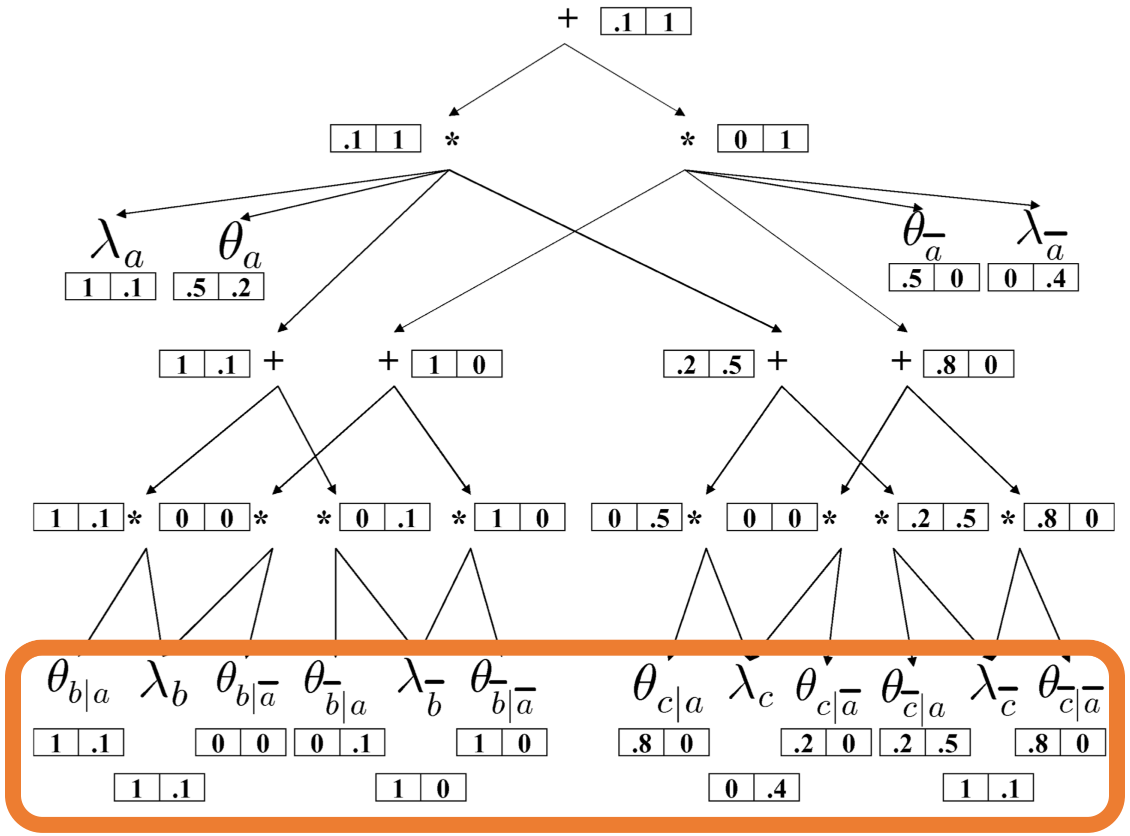


Darwiche, A Differential Approach to Inference in Bayesian Networks

Exact inference on AC to obtain quantum simulation

- Quantum simulation becomes tree traversal on AC

- ***<u>Quantum measurement outcomes are probabilistic evidence</u>***



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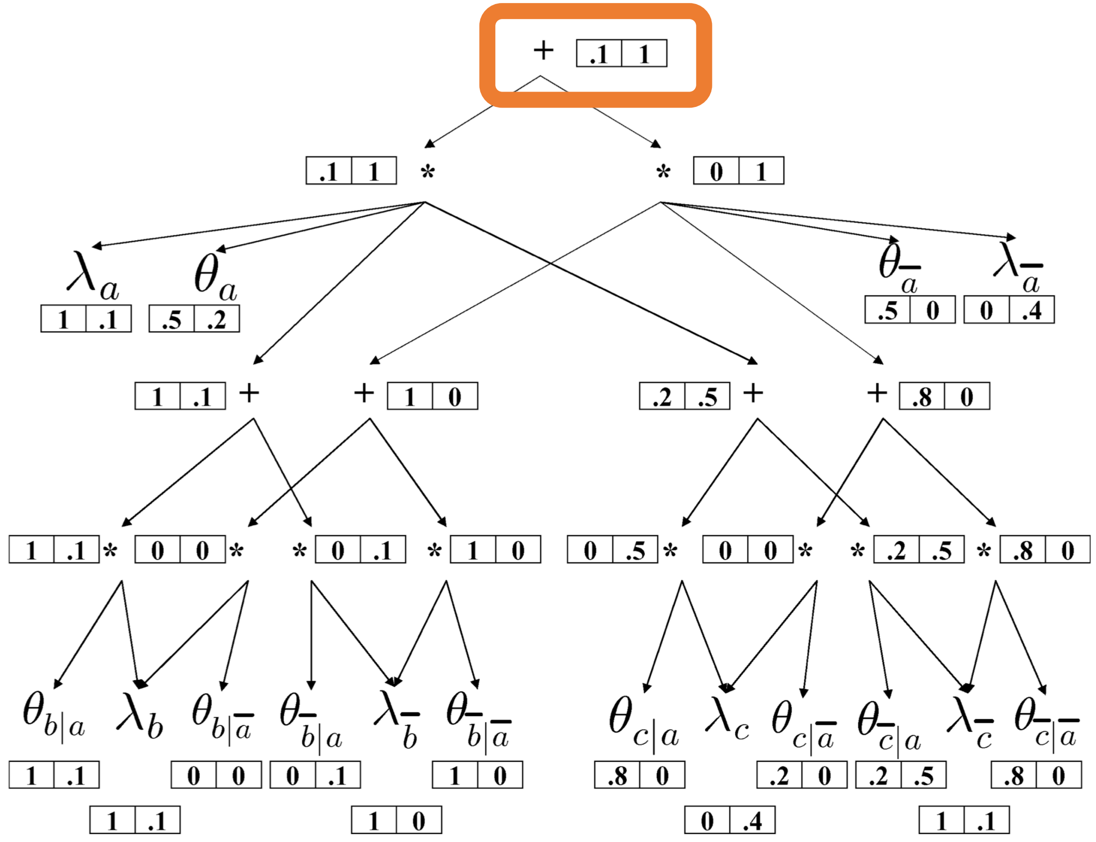
Exact inference on AC to obtain quantum simulation

- Quantum simulation becomes tree traversal on AC
- Quantum measurement outcomes are probabilistic evidence
- ***<u>Amplitude for given outcome comes from root node</u>***



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Result 1: It works!

With minimal modification, knowledge compilation exact inference can be repurposed for quantum simulation

- Can accurately simulate Pauli gates, CNOT, CZ, phase kickback, Toffoli, BV, Grover's, Shor's, random circuit sampling

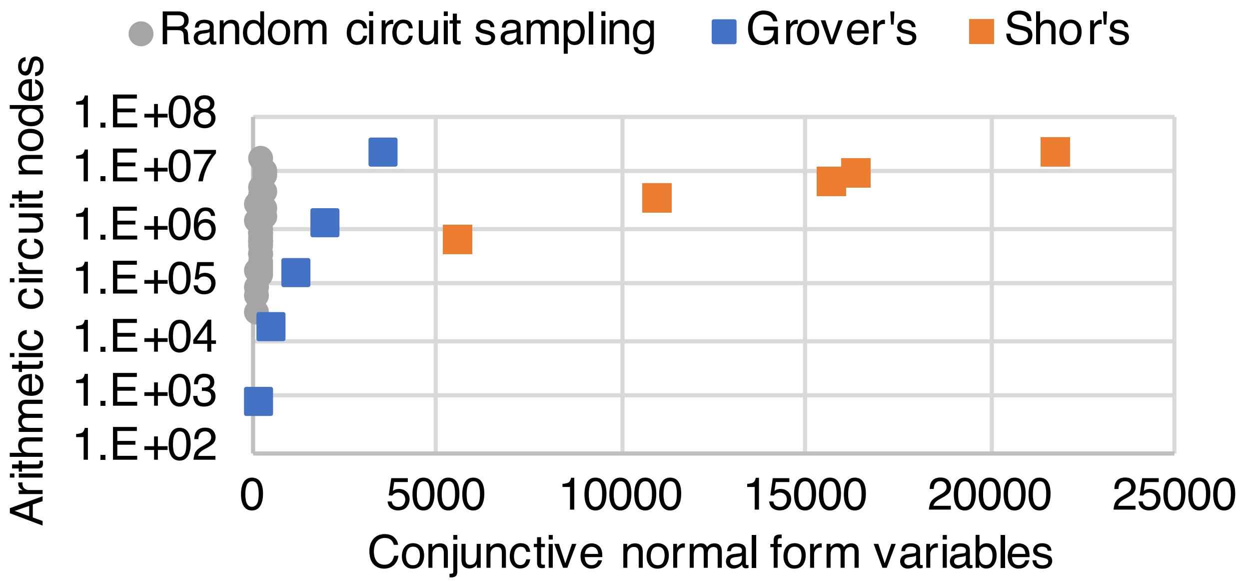
In general, works with exact inference methods

- E.g., variable elimination, weighted model counting

In general, fails with approximate inference methods

- E.g., Sampling, Markov chain Monte Carlo

Result 2: Ability to extract quantum circuit structure



	# qubits	# gates	AC file size
RCS	42	840	82 MB
Grover's	17	2460	530 MB
Shor's	13	12247	586 MB

(b) Problem size metrics for largest problem instances.

Y-axis: proportional to resource intensiveness

- Compilation/inference time, memory, storage

X-axis: proportional to the number of qubit states

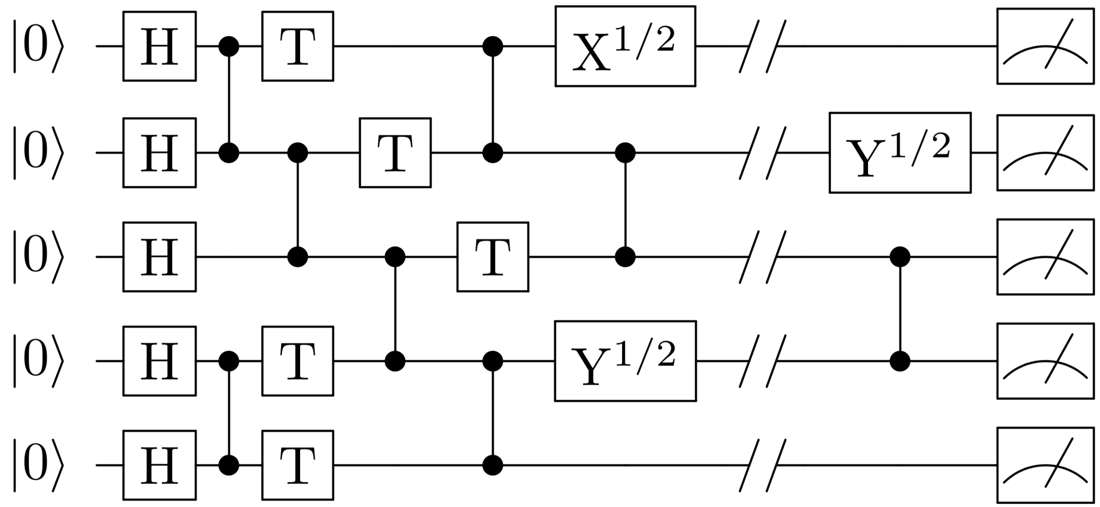
- Quantum circuit width × depth

Workloads taken from Scaffold

Result 3: More efficient repeated simulation with different measurement outcomes

Random circuit sampling

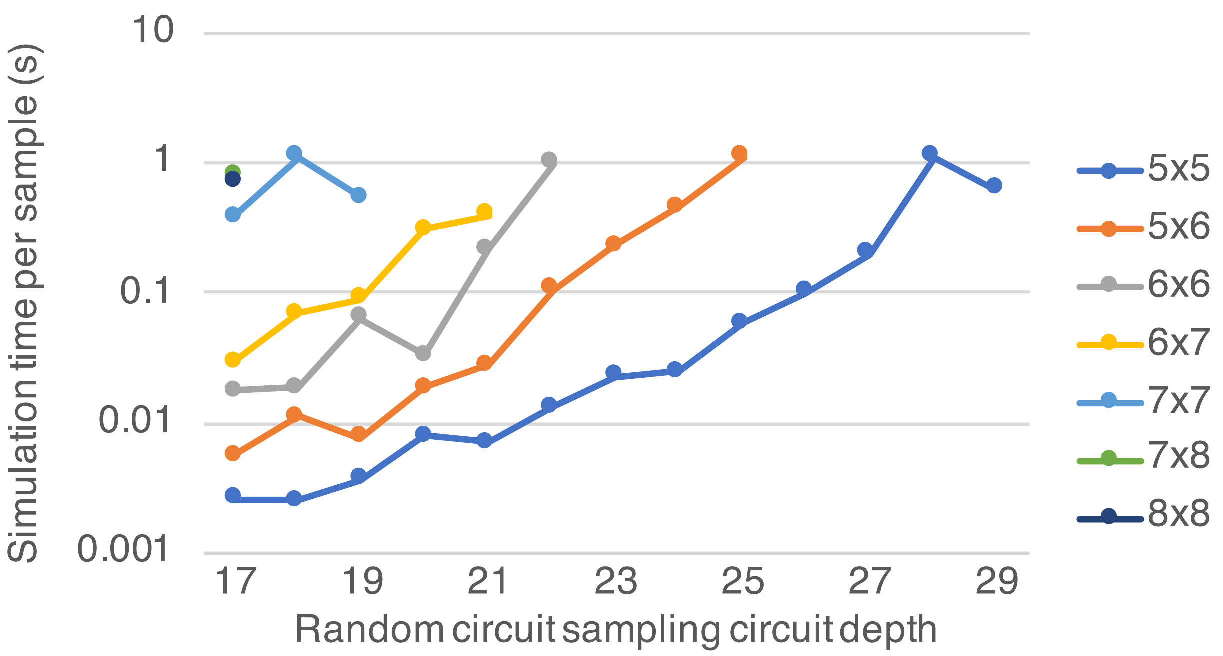
- Samples multiple measurement outcome assignments



Subject of intense competition

- Boixo et al. hinted reusing results between simulations may be useful

Result 3: More efficient repeated simulation with different measurement outcomes



First work where partial simulation results reused for RCS

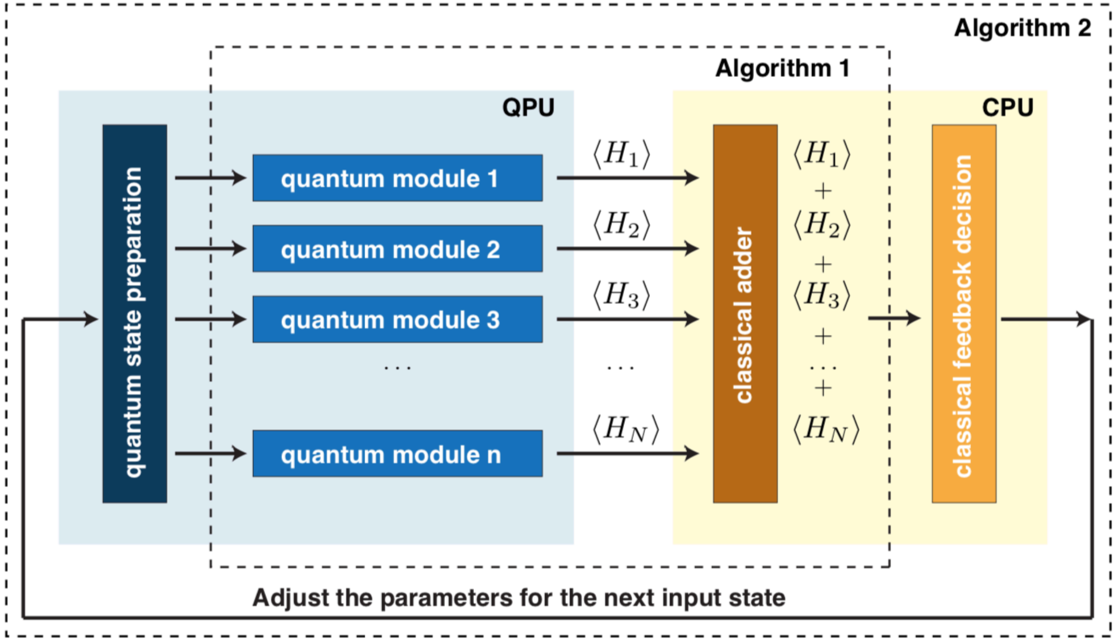
- Change of sampled measurement outcome only needs tree re-traversal

Up to about depth 29, ~20× speedup

- Against Boixo et al., on a workstation

Beyond depth 29, no structure to extract

Result 4: More efficient repeated simulation with different operator matrix parameters



Peruzzo et al., 2013

Toolchain stage	Computation time (s)
Quantum circuit to Bayesian network	0.372 ± 0.005
Bayesian network to CNF	1.219 ± 0.042
CNF to arithmetic circuit	12.077 (once)
Inference on AC	1.459 ± 0.350

Table 1: Time cost per toolchain stage for each of 88 iterations.

VQE Benchmark by Teague Tomesh, Princeton

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Teague Tomesh, Margaret Martonosi; Princeton

Members of the EPiQC team

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