Quantum emulators and scientific research

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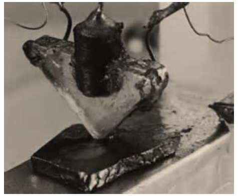
Will These Get Quantum 1.0?

Fredrik Bull’s
“sorting-recording-adding” machine
1919

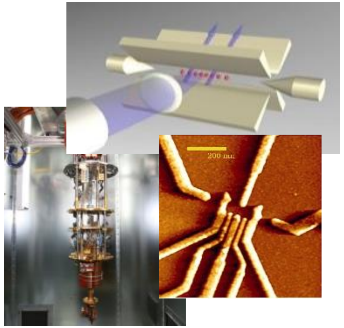
First quantum
revolution



Bull sequana
supercomputer

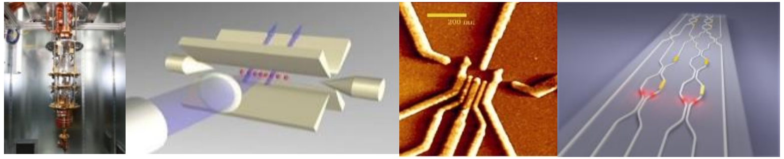
Will These Get Quantum 2.0?

Second quantum revolution



?

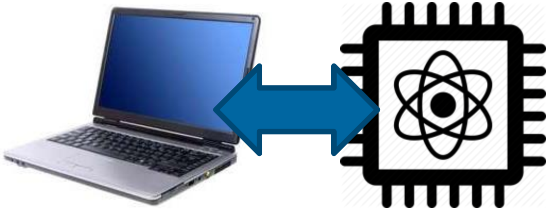
Why quantum hardware is not enough



- “Good qubits”: necessary… but not sufficient
- Beyond hardware:

Quantum algorithmics: very few known algorithms…
 - how to quickly program+validate new ideas?

NISQ era: before fault-tolerance
 - how to **compile** a program for a targeted hardware?
 - can we design **noise-resilient** algorithms?
 - **analog vs digital** approaches? …

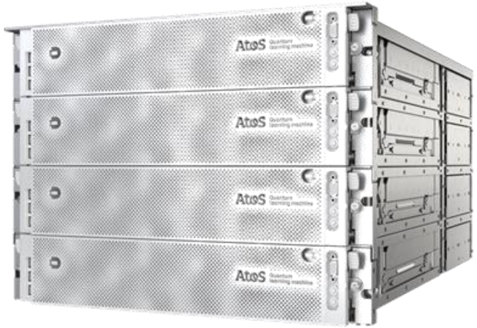


Quantum applications: “killer app(s)” yet to be found!
 - quantum-classical interface? (variational methods, error mitigation, pre- and post-treatment, parallelism…)

Need for (classical) programming/simulation/optimization tools

Outline

- **Modeling** quantum processors
- **Simulating** noisy quantum circuits with classical computers
- **Optimizing** noisy quantum circuits
- **Using** quantum processors to solve hard problems? Schwinger model example



Our collaborations

Quantum programming, classical simulation

BPI project Quantex (with Paris Saclay, CNRS-LORIA, CEA-LETI). *Quantum programming, hardware-acceleration for classical simulation of quantum circuits*

ANR SoftQPro (with Paris Saclay, CNRS-LORIA, CEA-LIST). *Numerical simulation of high-level quantum programming languages*.

CIFRE PhD thesis with Supélec/Saclay: *numerical techniques for quantum circuit generation*

Quantum algorithmics

QUANTERA QuantAlgo (with CNRS-IRIF, CWI-QuSoft, Cambridge, Univ. of Latvia, Univ. Libre de Bruxelles). *Machine Learning, exploration of use cases.*

ANR QuData (with CNRS-IRIF, Paris-Sorbonne, CNRS-LABRI). *Assessment of industrial use cases*.

CIFRE PhD thesis with IRIF: *algorithms for Quantum Machine Learning.*

Quantum hardware

EU-Flagship project AQTION (with Univ. Innsbruck (Blatt group), Oxford, ETHZ, Mainz, Fraunhofer, Swansea, Toptica). *Programming frontend, compilation, industrial use cases*

Chaire industrielle NASNIQ (with CEA-DRF Quantronics lab). *Computational architecture, noise models*

Merlion project Siliquon qubits (with CNRS-Néel, Singapore Institute of Quantum Computing). *Noise simulation of Si Qubits*

Analog quantum simulation

EU-Flagship PASQUANS Flagship project (with Institut d’Optique, Univ. Innsbruck (Zoller group), ETHZ, Univ Munich, LKB, Univ Strathclyde, Univ Ulm, Univ Padova, Univ Heidelberg).

WP leader of applications

1

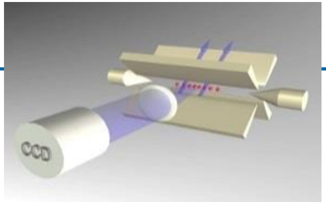
Modeling quantum processors

All qubits are not created equal

Superconducting qubits

- Coupled anharmonic oscillators (Josephson junctions)

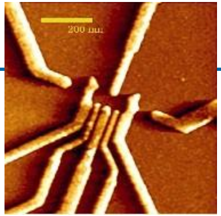
- Gates ~ 200 ns, coherence ~ 50 μs: 250 gates, 1-f=0.002
- ~10 entangled qubits, ~50 qbit chips announced
- Limited connectivity
- Limited scalability (need very precise calibration)?



Trapped ions

- Entangle internal degrees of freedom via motional mode

- Gates ~ 50 us, coherence ~ 200 ms: 4k gates, 1-f = 0.05
- All-to-all connectivity
- ~ 15 entangled qubits
- Limited scalability (large crystal: vibration modes…)?
- Alternatives: shuttling…



(etc)

Quantum dots

- Entangle electron spins via exchange J

- 1 and 2-qbit gates demonstrated… not more!
- Leverage CMOS technology: Scalable?

Yet, we want to be able to program them in a hardware-agnostic way.

How to describe noisy quantum computers?

- Quantum processors: fragile quantum systems in classical environment
  - Noise: -> mixed quantum state: **density matrix $\boldsymbol{\rho}$** (instead of $|\psi\rangle$)

    $2^n \times 2^n$ matrix instead of 2^n vector! (n: number of qbits)

- **Several approaches to describe noise**
  - Continuous-time approach: master equation

    e.g Lindblad master equation (Markovian noise: memory-less env.)

$$i\frac{d\rho}{dt} = [H,\rho] + i\sum_n \gamma_n \left(L_n \rho L_n^+ - \frac{1}{2}\{L_n^+ L_n, \rho\} \right)$$

    - requires knowledge of γ_n, L_n
    - can reduce cost to 2^n: quantum trajectories
    - continuous time: not very suitable for optimized compilation:

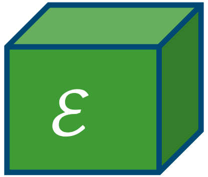
we would like to adopt **discrete** description

Building blocks: Noisy gates

- Quantum state evolution via ‘quantum channels’ or ‘CPTP maps’

$$\rho \to \mathcal{E}(\rho)$$

  - **complete positivity** (CP): “unitary total evolution”
  - **trace preservation** (TP): “no leakage”



- Several representations of quantum channels:
  - **Kraus representation**:

$$\mathcal{E}(\rho) = \sum_k E_k \rho E_k^{+}$$

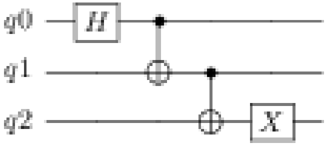
  - **Pauli transfer matrix** (PTM): (Chow et al ‘12)

$$\overrightarrow{\mathcal{E}(\rho)} = \boldsymbol{R} \cdot \vec{\rho}$$

how to specify noisy gates for a given hardware?

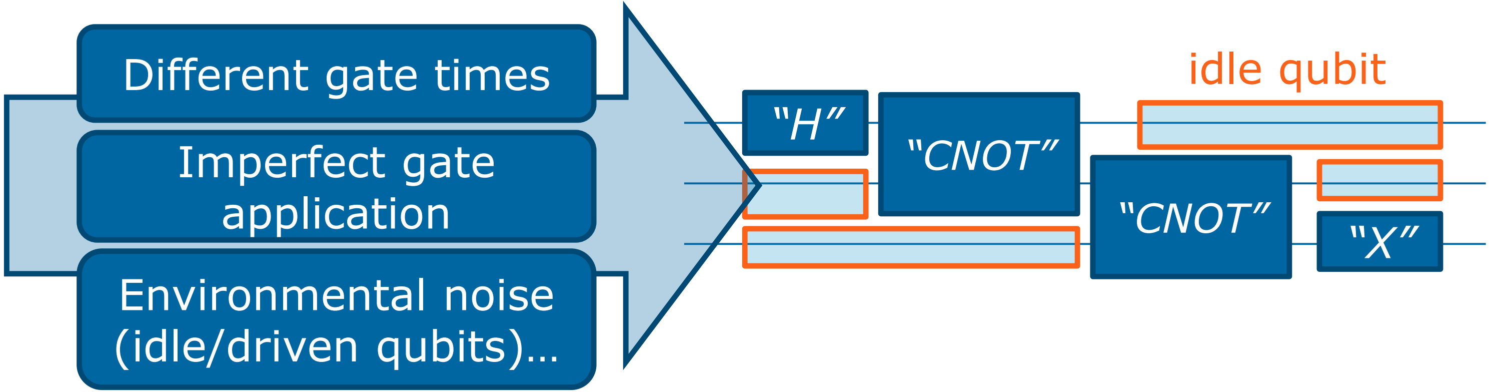
Discrete modeling of noise

Ideal circuit



Hardware model

Noisy circuit


Different gate times

Imperfect gate application

Environmental noise (idle/driven qubits)…

- Modular, hence **scalable** approach
- Captures **large variety of noises** (incl. spatially correlated, crosstalk, leakage…)

- **Caveat**: does not capture all memory effects

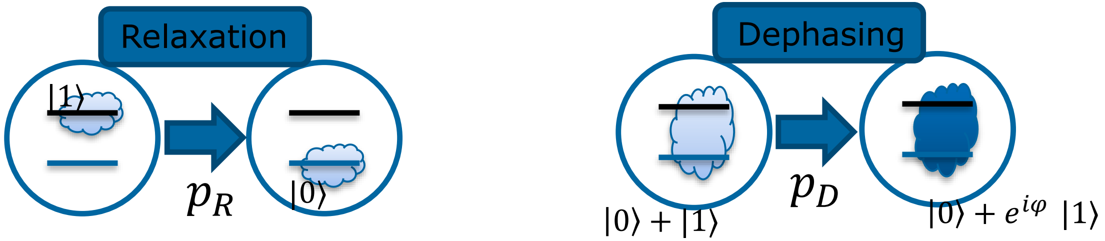
What do the boxes look like?

Textbook noise models…

- **Bit-flip noise**: $\mathcal{E}(\rho) = (1 - p_F)\rho + p_F X\rho X$
  "flip bit with probability p_F"
  Two Kraus operators: $E_1 = \sqrt{1 - p_F}\,\mathrm{Id}$ and $E_2 = \sqrt{p_F}\,X$

see e.g. Nielsen & Chuang

- **Relaxation** (aka amplitude damping) **and dephasing:**

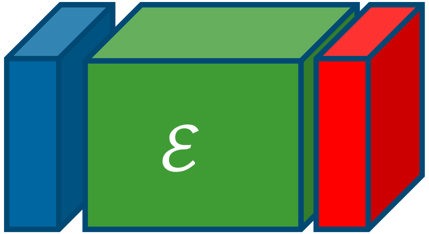


Challenge: what is p_F, p_R, p_D … for a given hardware?
Are there other important types of noise?

… and more ‘ab initio’ approaches: tomography

- Characterize $\mathcal{E}(\rho)$: **“process tomography”**
- Two complementary strategies:

prepare
($\geq 4^{nqbits}$)
basis states



project on
basis
states

Experiment/phenomenology

- **Quantum process tomography**: 16 circuits for 1-qbit gate, 256 for 2-qbit… (x lots of shots)
- **Gateset tomography**: consistent treatment of “SPAM” error

Merkel et al 2013

Advantage: phenomenological (“black box”) approach

Numerics

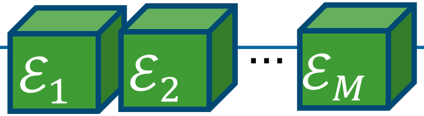
- Write **Hamiltonian model** for given operation
- Solve **Schrödinger/master equation** for all inputs

Advantage: inputs are usually experimentally accessible (microscopic) parameters.

2

Classical simulation (emulation) of ideal and noisy circuits

What we want to compute



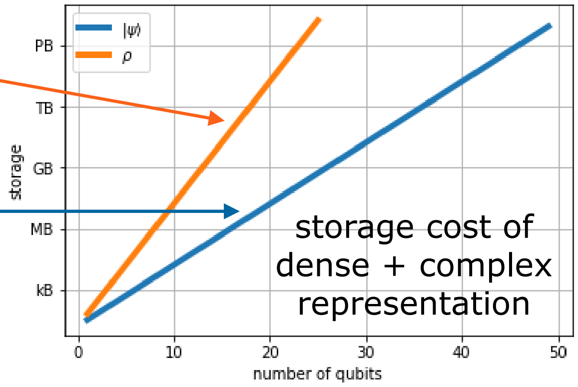
- Final density matrix after M operations:

$$\mathcal{E}(\boldsymbol{\rho}) = \sum_{k_M}\left(E_{k_M}^{(M)} \dots \left(\sum_{k_1} E_{k_1}^{(1)}\boldsymbol{\rho}E_{k_1}^{(1)\dagger}\right)\dots E_{k_M}^{(M)\dagger}\right)$$

  - Large memory requirement ($2^n \times 2^n$ matrices)

- Compare to **"ideal" quantum computation**:
  - Pure state $\boldsymbol{\rho} = |\psi\rangle\langle\psi|$…: "only" 2^n complex numbers
  - Only one Kraus op.: $\mathcal{E}(\boldsymbol{\rho}) = U\boldsymbol{\rho}U^\dagger$:

    unitary evolution $U_M \dots U_1|\psi\rangle$



storage cost of dense + complex representation

- Both require advanced numerical techniques **to reach few tens of qbits**

Ideal circuit simulation

Unitary evolution $|\psi_f\rangle = U_M \dots U_1 |\psi_i\rangle$

- **"Brute-force" simulation:**
  - store 2^n amplitude vector:

$$|\psi\rangle = \sum_{b_1..b_N} a_{b_1..b_N} |b_1..b_N\rangle$$

$a_{b_1 b_2 b_3 b_4} =$

  - up to 40-41 qubits

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- **Stabilizer simulation**
  - Only “Clifford” gates: can represent state with $O(n^2)$ cost
  - can simulate >1000 qubits
  - Extensions for Clifford+T…

Gottesman & Knill

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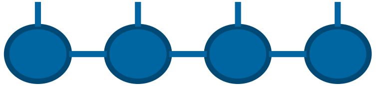
- **Using entanglement structure: Matrix product state (and tensor networks)**
  - MPS representation (4 qbits):



see e.g
Schollwöck ‘10,
Orus ‘14

  - physics insights from “bond dimension”
  - can simulate $\gg$ 40 qubits

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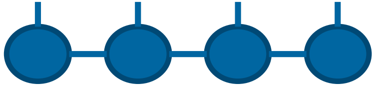

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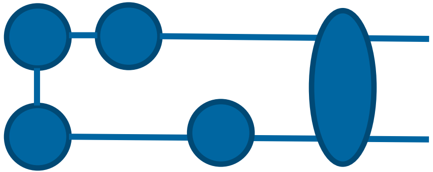
Gottesman & Knill

- **Tensor network contraction**
  - space+time network (2 qbits + 4 gates)



  - challenge: find fast contraction order

Noisy simulation

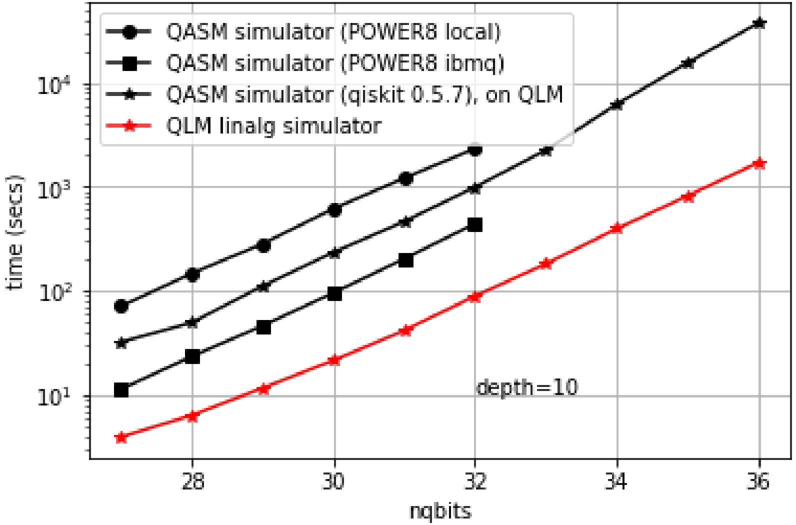
- Density-matrix evolution: $\mathcal{E}(\boldsymbol{\rho}) = \sum_{k_M} \left(E_{k_M}^{(M)} \dots \left(\sum_{k_1} E_{k_1}^{(1)} \boldsymbol{\rho} E_{k_1}^{(1)\dagger} \right) \dots E_{k_M}^{(M)\dagger} \right)$
  - ~OK for <20 qubits
- More qubits: rewrite as sum over “**trajectories**”

$$\mathcal{E}(\boldsymbol{\rho} = |\boldsymbol{\psi_0}\rangle\langle\boldsymbol{\psi_0}|) = \sum_{k_1..k_M} E_{k_M}^{(M)} \dots E_{k_1}^{(1)} |\boldsymbol{\psi_0}\rangle\langle\boldsymbol{\psi_0}| E_{k_1}^{(1)\dagger} \dots E_{k_M}^{(M)\dagger}$$

- One trajectory $k_1 .. k_M$: apply “gates” $E_{k_1}^{(1)} \dots E_{k_M}^{(M)}$ to $|\psi_0\rangle$
  - Reduction of storage cost… but exponential #trajectories
- **Stochastic sampling** over all possible trajectories

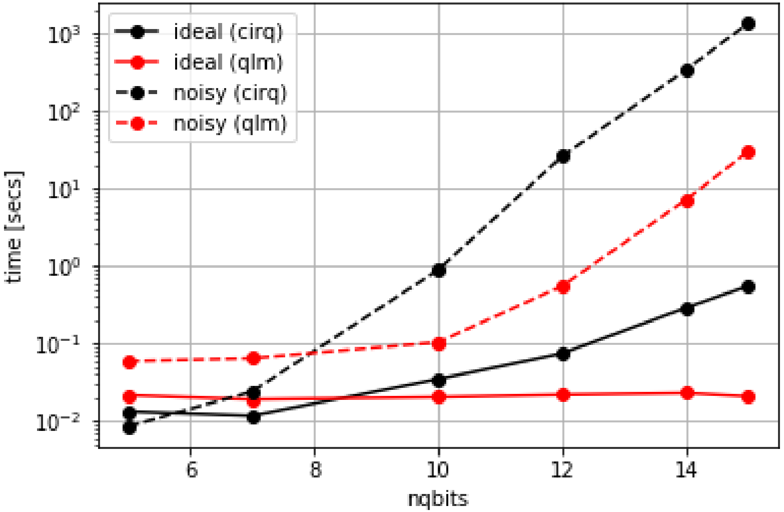
Speed comparison

Atos QLM vs IBM Qiskit simulator
Ideal simulation
'Quantum volume' benchmark circuit



QLM: **qat.linalg** simulator
IBM POWER8 benchmark data from
www.ibm.com/blogs/research/2018/05/quantum-circuits

Atos QLM vs Google cirq simulator
Ideal + noisy simulation
H+CNOT circuit



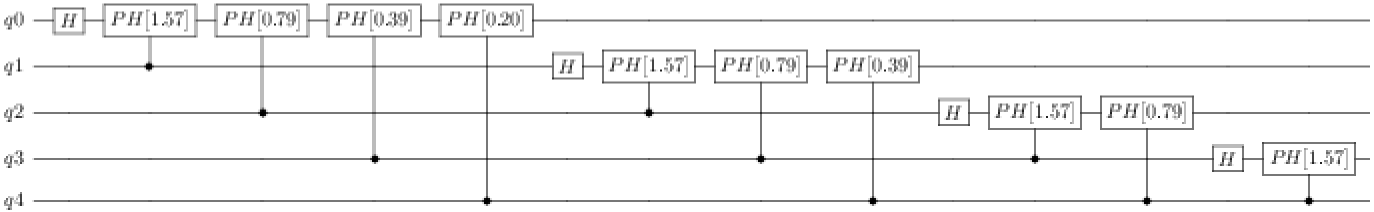
QLM: **qat.linalg and qat.noisy** simulator

2

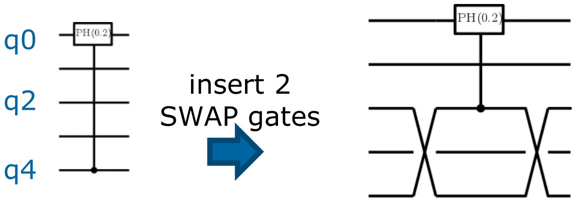
A word on compilation

Compilation under connectivity constraints

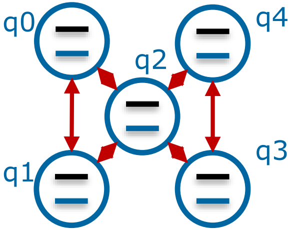
- Concrete example: Quantum Fourier Transform



- Compilation for connectivity:



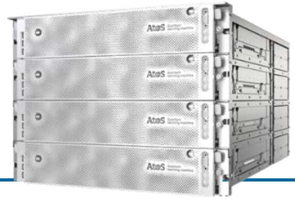
insert 2
SWAP gates



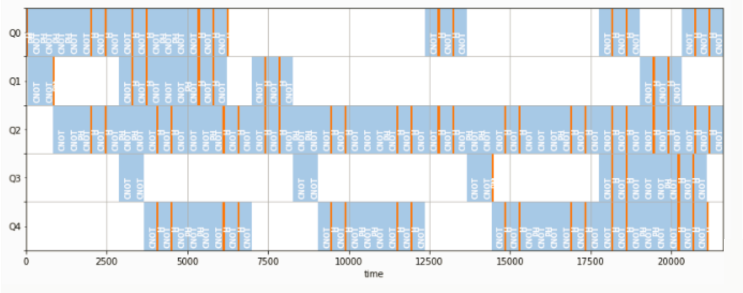
(here: undirected graph)

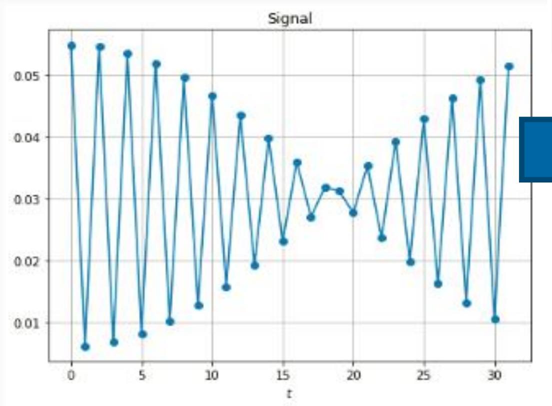
Large gate count overhead!

Example: Quantum Fourier Transform on 5 noisy qubits

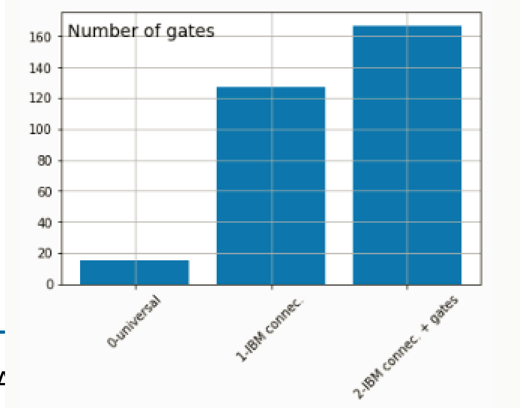


Decoherence noise only
on idle qubits,
perfect gates

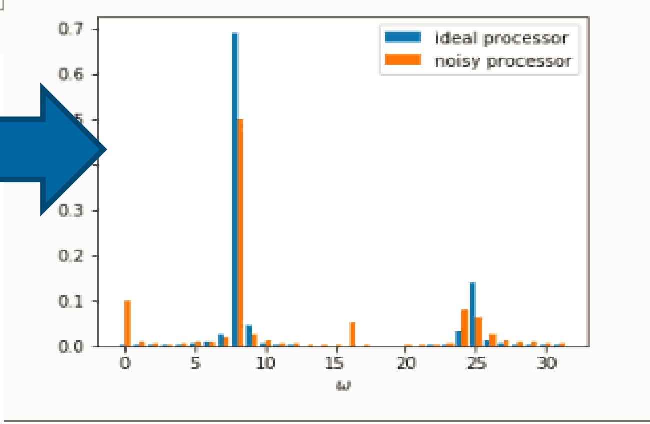




compilation, simulation



Typical noise
parameters
for IBM
device

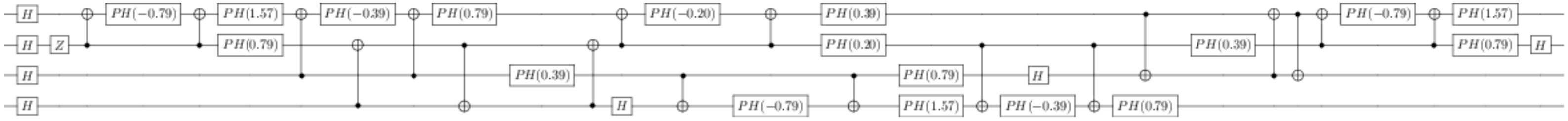


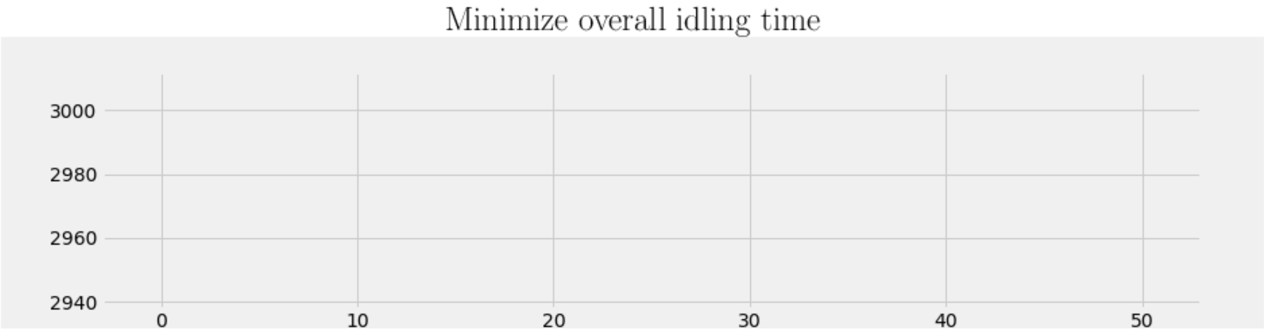
3

Optimizing quantum circuits

Example 1: Minimization of the total idling time

- Start from QFT compiled for connectivity & gateset
- Use **commutation patterns** to reduce **total idling time**
- Minimization via (classical) **simulated annealing**





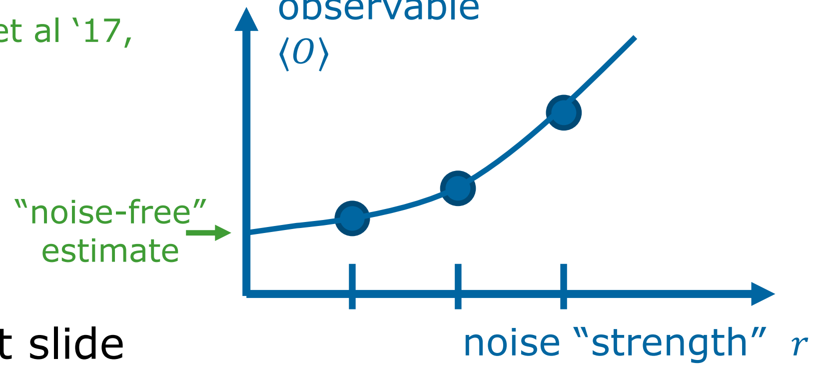
total idling time

annealing steps

Example 2: Error mitigation

- Error mitigation: before full-fledged quantum error correction

- Several methods, e.g   Li & Benjamin ‘17, Temme et al ‘17, Endo et al ‘17…
  - **Zero-noise extrapolation**: artificially enhance noise and extrapolate
  - **Quasiprobability error mitigation**: next slide



Software-based methods requiring
good control and/or knowledge of hardware

Quasiprobability error mitigation

(Temme et al `17, Endo et at `17)

- Observable: $\langle O\rangle = \ll O|\mathcal{E}_M \dots \mathcal{E}_1|\rho \gg \neq \langle O^{(0)}\rangle = \ll O^{(0)} \left|\mathcal{E}_M^{(0)} \dots \mathcal{E}_1^{(0)}\right| \rho^{(0)} \gg$

  with $\mathcal{E}_i$ ($\mathcal{E}_i^{(0)}$): imperfect (perfect) hardware operations

- Two steps:

1. **Linear decomposition** of perfect ops. on hardware ops.:

$$\mathcal{E}_i^{(0)} = \sum_{j_i} q_{j_i}^{(i)} \mathcal{E}_{j_i}$$

   Obtain sum over (exponentially many) "trajectories":

$$\langle O^{(0)}\rangle = \sum_{j_1 \dots j_M} q_{j_1}^{(1)} \dots q_{j_M}^{(M)} \ll O|\mathcal{E}_{j_M} \dots \mathcal{E}_{j_1}|\rho \gg$$

2. **Stochastic sampling** over trajectories

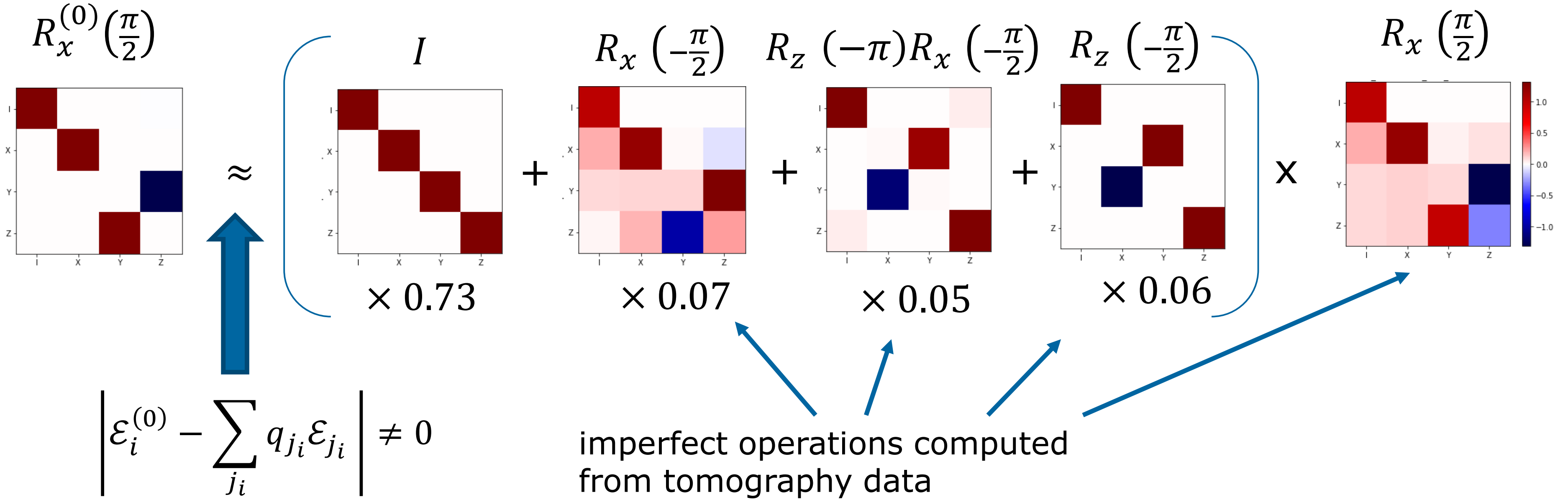
Caveats:

1) $\mathcal{E}_{j_i}$ should form a basis! (incl. non-unitary ops)

2) q_j not necessarily positive: "quasiprobabilities" (-> increased variance: 'sign problem')

Example of decomposition

- Using gateset tomography data on IBM QX4:



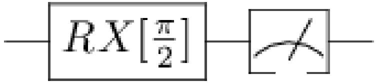
$$R_x^{(0)}\left(\frac{\pi}{2}\right) \approx \left(I \times 0.73 + R_x\left(-\frac{\pi}{2}\right) \times 0.07 + R_z(-\pi)R_x\left(-\frac{\pi}{2}\right) \times 0.05 + R_z\left(-\frac{\pi}{2}\right) \times 0.06 \right) \text{x}\; R_x\left(\frac{\pi}{2}\right)$$

$$\left| \mathcal{E}_i^{(0)} - \sum_{j_i} q_{j_i}\mathcal{E}_{j_i} \right| \neq 0$$

imperfect operations computed from tomography data

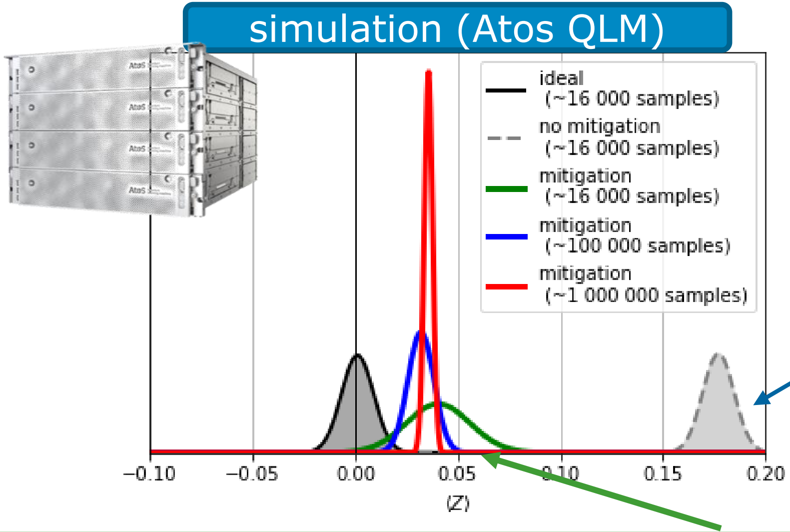
Comparison: noisy simulation vs. experiment

- Example circuit:

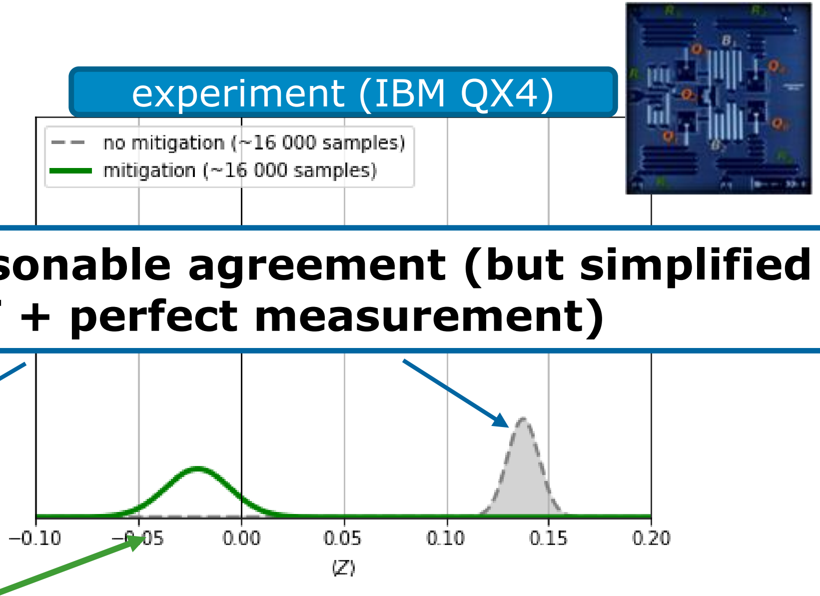


- Output state is (supposedly) $\propto (|0\rangle - i|1\rangle)$. Observable: $\langle Z \rangle = 0$
- Preliminary results:

simulation (Atos QLM)



experiment (IBM QX4)



reasonable agreement (but simplified GST + perfect measurement)

much more accurate, but still biased (limited operation set $\left|\mathcal{E}_i^{(0)} - \sum_{j_i} q_{j_i}\mathcal{E}_{j_i}\right| \neq 0$**)**

4

Potential applications of NISQ computers

Applications

- **Natural target: Quantum simulation** (equilibrium and dynamics)
  - quantum chemistry
  - condensed-matter physics

$$H|\psi\rangle = E|\psi\rangle \qquad i\frac{d|\psi\rangle}{dt} = H(t)|\psi\rangle$$

exponential cost with system size (or Monte-Carlo sign problem)

- **(Classical) Combinatorial optimization problems**
  - e.g clustering

  - Minimize cost function… which can be discretized -> Boolean function $C(z_1, \ldots, z_N)$ (classical Ising Hamiltonian <-> spin glass problems)

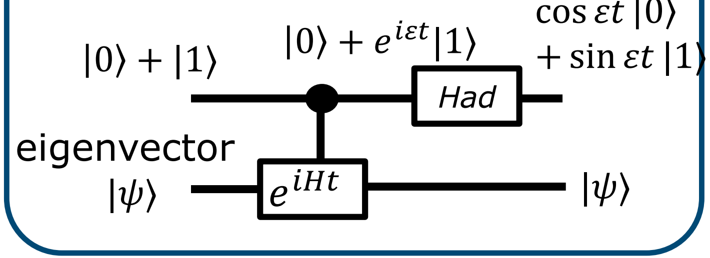
- **And also** (later): factoring (Shor), quantum machine learning, database search (Grover)…

Two approaches to quantum simulation

- **Analog approach**
  - Ultra-cold atoms, trapped ions, Rydberg atoms…
    - Good (global) control of a given Hamiltonian
  - Superconducting circuits: quantum annealing (d-wave)
    - Find ground state of (classical) Ising model

- **Digital approach:** gate-based (universal)
  - Superconducting circuits, trapped ions…
  - **Long term:**
    - **Quantum phase estimation:** find eigenvalue of an eigenvector: $\mathrm{e}^{iHt}|\psi\rangle = e^{i\varepsilon t}|\psi\rangle$
    - Requires very deep (long) quantum circuits: state preparation, trotterization…

"Phase kick-back"



Hybrid variational algorithms

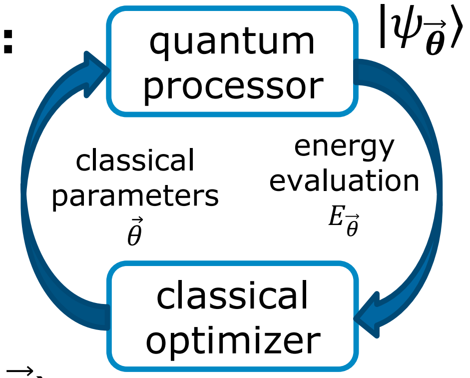
- **NISQ (Noisy intermediate scale quantum) computers:**
  - small number of qubits + short coherence times

- **Variational Quantum Simulation** (VQE, Peruzzo ’14, VQS, Kokail ’19…)

Goal: find ground state energy of Hamiltonian H

1. Choose (smart) variational ansatz $|\psi_{\vec{\boldsymbol{\theta}}}\rangle$ (with polynomial $\vec{\boldsymbol{\theta}}$)

   e.g (unitary) coupled cluster $\left|\psi_{\vec{\boldsymbol{\theta}}}\right\rangle \propto e^{i\sum \theta c^{+}c+h.c}|\phi_{HF}\rangle$
2. Find (short) quantum circuit / hamiltonian that creates $\left|\psi_{\vec{\boldsymbol{\theta}}}\right\rangle$
3. Measure variational energy $E_{\vec{\theta}} = \left\langle\psi_{\vec{\boldsymbol{\theta}}}|H_T|\psi_{\vec{\boldsymbol{\theta}}}\right\rangle$ with $H_T = \sum_\alpha \lambda_\alpha P_\alpha$, P_α product of Pauli operators
4. Use classical optimizer to find optimal $\vec{\theta}^*$



quantum processor

$|\psi_{\vec{\boldsymbol{\theta}}}\rangle$

classical parameters $\vec{\theta}$

energy evaluation $E_{\vec{\theta}}$

classical optimizer

Applications of variational quantum algorithms

- Quantum chemistry
  - Many small molecules have been studied (H2, LiH, …)
  - Well-known variational states: unitary coupled cluster (UCC), etc.

- Combinatorial optimization
  - Quantum approximate optimization algorithm (QAOA): special ansatz inspired from quantum annealing

- **Focus:** Variational quantum algorithms for **quantum field theory**?
  - Lattice QCD: a gauge theory plagued by Monte-Carlo sign problem in interesting regimes (hot quark-gluon plasma, neutron stars…)
  - Here, take Schwinger model (1+1-dim QED) as proxy for lattice QCD physics

Challenge I: translate problem to quantum computer language

- (Kogut-Susskind) **fermions**… in **spin**/qbit-based quantum computer?
  - Jordan-Wigner transformation

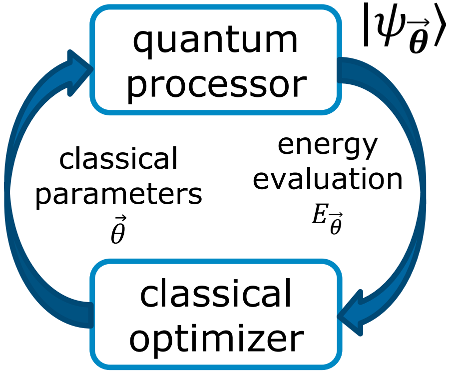
- infinite gauge degrees of freedom… in finite-dim quantum computer?
  - Use Gauss law to eliminate gauge d.o.f -> traded for exotic **long-range spin-spin interactions**

- **Final Hamiltonian:**

$$H_T = \sum_j \sigma_j^+ \sigma_{j+1}^- + h.c + \frac{m}{2} \sum_j (-)^j \sigma_j^z + \frac{g}{4} \sum_j \left(\sum_{l \leq j} \sigma_l^z + (-)^l \right)^2$$

with mass m, coupling g

Challenge II: Experimental realization



quantum processor

$|\psi_{\vec{\theta}}\rangle$

energy evaluation $E_{\vec{\theta}}$

classical optimizer

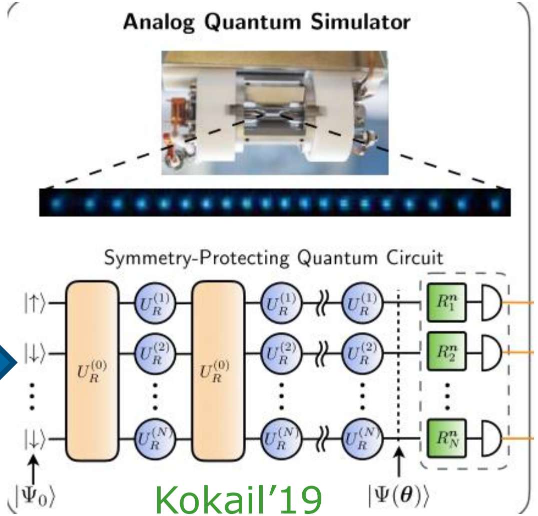
classical parameters $\vec{\theta}$

- Implementation of

$$H_T = \sum_j \sigma_j^+ \sigma_{j+1}^- + h.c + \frac{m}{2}\sum_j (-)^j \sigma_j^z + \frac{g}{4}\sum_j \left(\sum_{l\leq j} \sigma_l^z + (-)^l\right)^2$$

- Many recent publications:
  - digital computation with 4 ions (Martinez et al Nature ’16), 5 SC qubits (Klco et al PRA ’18), …
  - analog computation with 20 ions (Kokail et al Nature ‘19)

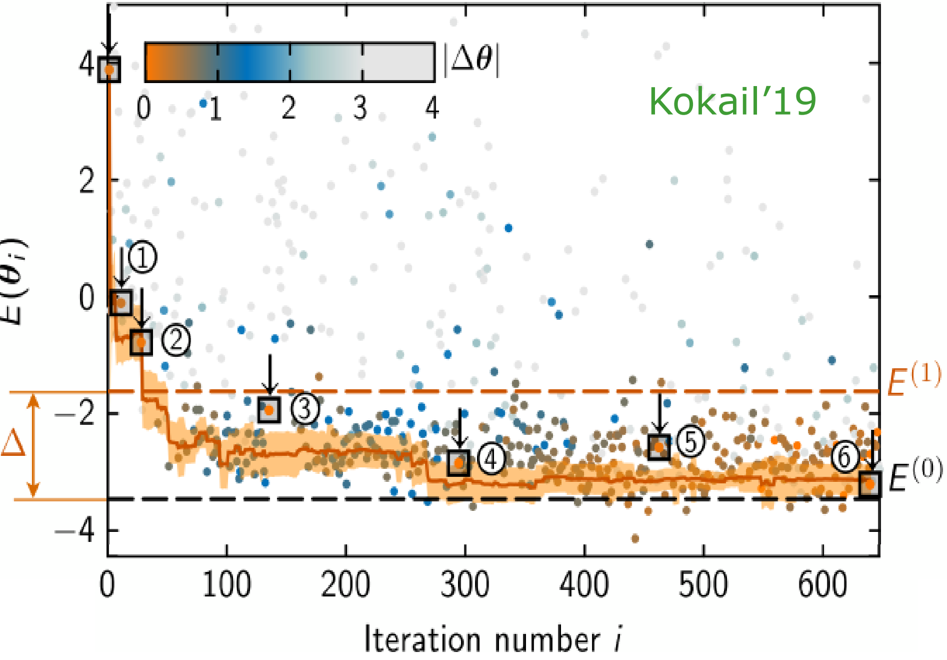
- **Here**: focus on analog computation
  - Preparation of $|\psi_{\vec{\theta}}\rangle$ with “resource” Hamiltonians H_R
  - Bonus: H_T and H_R share symmetries



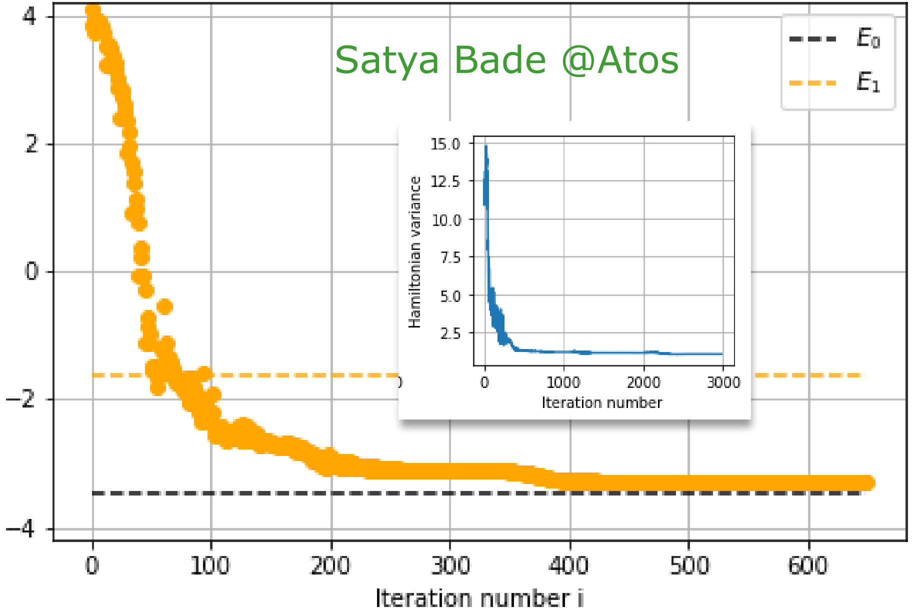
Kokail’19

Experimental results and simulation

- Experimental result (Nions=8):



- Our simulation (Nions=8):

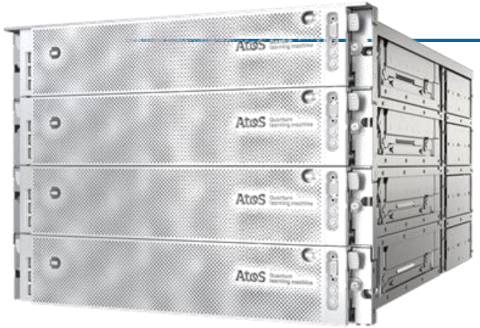


5

Conclusion: a dedicated platform for quantum simulation and computation

A platform to research and experiment quantum software

The Atos Quantum Learning Machine



QLM: a special-purpose classical simulator

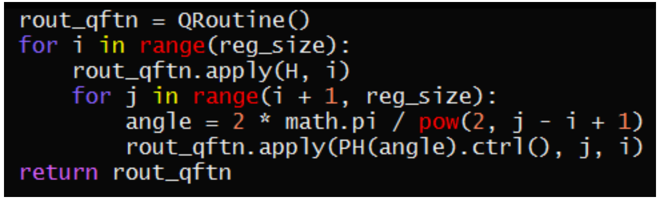
quantum programming libraries

quantum routines (QFT…), oracles, custom & abstract gates…

circuit optimization

connectivity constraints, graph-based optimization…

c++, python, jupyter, …



```
rout_qftn = QRoutine()
for i in range(reg_size):
    rout_qftn.apply(H, i)
    for j in range(i + 1, reg_size):
        angle = 2 * math.pi / pow(2, j - i + 1)
        rout_qftn.apply(PH(angle).ctrl(), j, i)
return rout_qftn
```

hybrid quantum-classical programming

perfect circuit simulation

at least 40 “logical” qubits

Various methods: full vector state, Matrix Product State, stabilizer, sum-over-histories…

noisy simulation

noise and hardware models

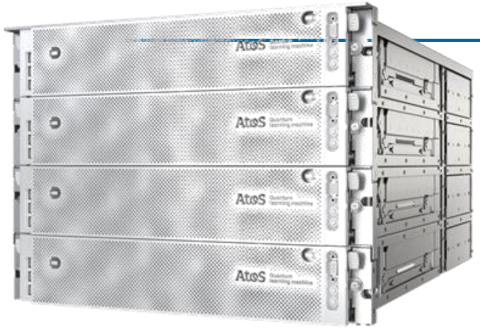
Various methods: full density matrix, Matrix Product Operator, quantum trajectories

application libraries

Spin/Fermionic models and translation to circuits
VQE + QAOA (optimizers…)

A platform to research and experiment quantum software

The Atos Quantum Learning Machine



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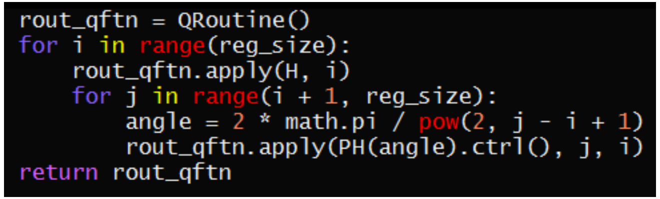

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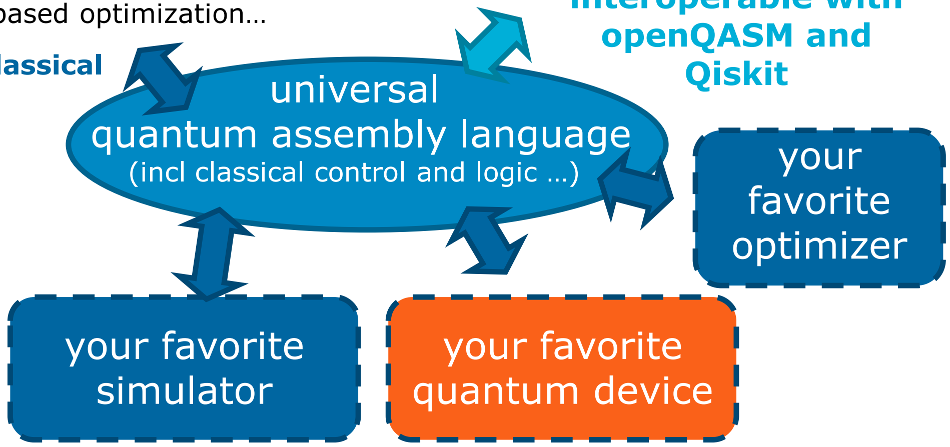

interoperable with openQASM and Qiskit

universal
quantum assembly language
(incl classical control and logic …)

your favorite optimizer

your favorite simulator

your favorite quantum device

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Thanks

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