Simulation, optimization and applications of near-term quantum computers Thomas Ayral, Atos Quantum Lab

December 3rd, 2019



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Bridging the gap

Many theoretical ideas

- Quantum algorithmics
 Very few known
 algorithms (+need many
 good quality gates & many qubits)
- NISQ: Hybrid quantum classical programs
 - Variational Quantum Eigensolver and Simulator (VQE, VQS)
 - Error mitigation...

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Many hardware implementations



- Different connectivities
- Different gatesets
- Different gate qualities/durations
- Different readout errors
- Different coherence times
- Different scalability
 - Analog vs digital
 - Adiabatic vs diabatic

No

killer app



Outline

Simulation

efficiently simulating the (imperfect) behavior of each platform

Optimization

developing quantum programs in a hardware-agnostic way... but suitably optimized for target platform

Applications

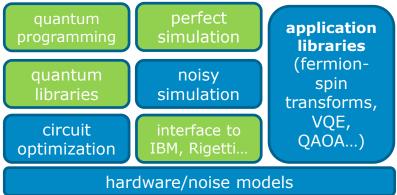
Focus: Schwinger model energy with variational algorithms

Atos Quantum Learning Machine



a dedicated quantum programming platform

myQLM: "QLM lite", free!





Atos quantum: worldwide...



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... and at home: 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 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 Oubits

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.*

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





Simulation efficiently simulating the (imperfect) behavior of each platform

The quantum Fourier transform: theory...

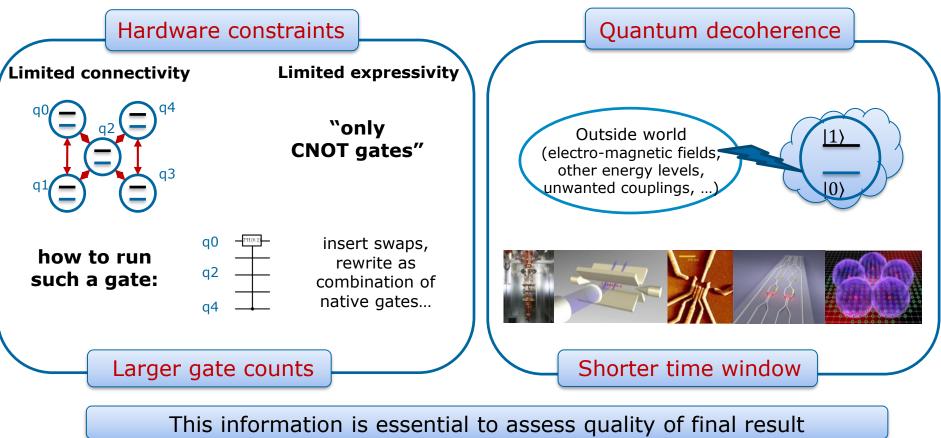
state preparation \Rightarrow computation: apply quantum gates \Rightarrow final step: measurement

- In theory: exponential speedup (over fast Fourier transform)
- Key ingredient of Shor's factoring algorithm

Promise of huge speedups... if "ideal" quantum computer

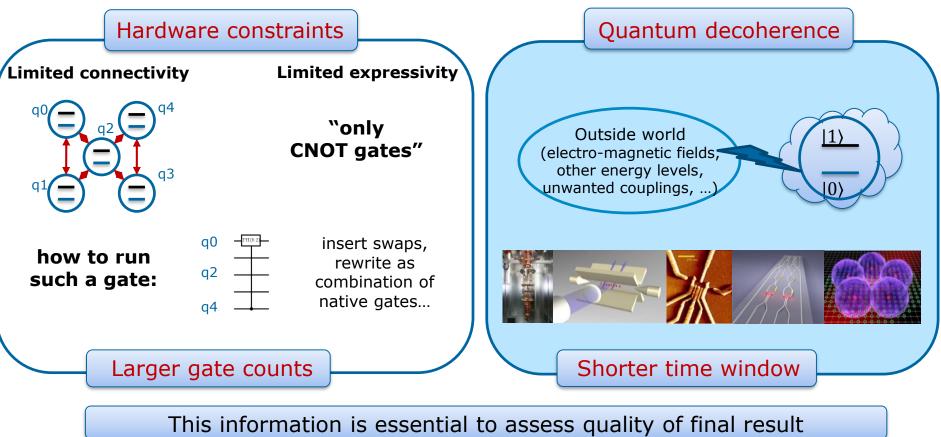


... and practice



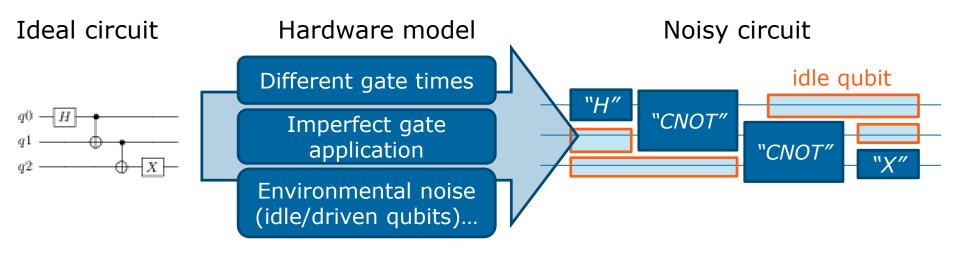


... and practice





Discrete modeling of noise



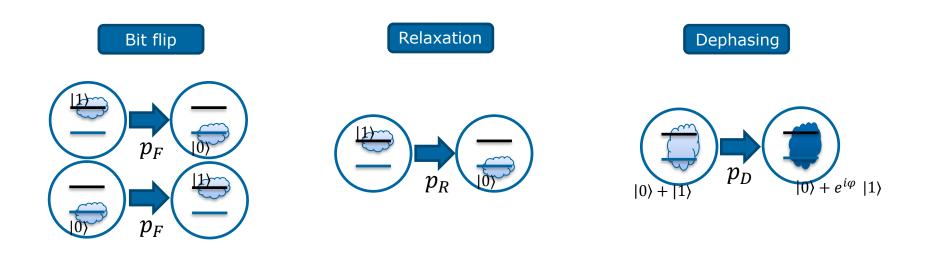
- Modular, hence scalable approach
- Can capture large variety of noises (incl. spatially correlated, crosstalk, leakage...)
- Caveat: does not capture all memory effects

What do the boxes look like?



Textbook noise models...

see e.g. Nielsen & Chuang



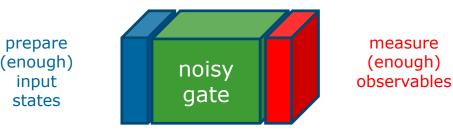
Challenge: what is p_F, p_R, p_D ... for a given hardware? Are there other important types of noise?

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... and more 'ab initio' approaches: tomography

- Characterize noise processes:
 "process tomography"
- Two complementary strategies:



Experiment (phenomenology)

- Quantum process tomography: assume known state preparation & measure (aka SPAM) (!)
- Gateset tomography: consistent handling of SPAM error Merkel et al / Blume-Kohout et al 2013

Advantage: phenomenological ("black box") approach

Numerics (microscopic model)

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

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



Ideal vs Noisy quantum computation

Ideal circuit simulation

- Quantum state:
 - pure state $|\psi\rangle$
 - generically: 2ⁿ
 complex numbers
- Gates:
 - unitary operators *U* acting on subsets of qubits
- Memory footprint

Noisy simulation

- Quantum state:
 - mixed state $\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i |$
 - generically: $2^n \times 2^n$ complex numbers

Gates:

 linear, "CPTP" maps ε(ρ) (completely positive, trace preserving)

Simulation:

 $\left|\psi_{f}\right\rangle = U_{M}\ldots U_{1}|\psi_{i}\rangle$

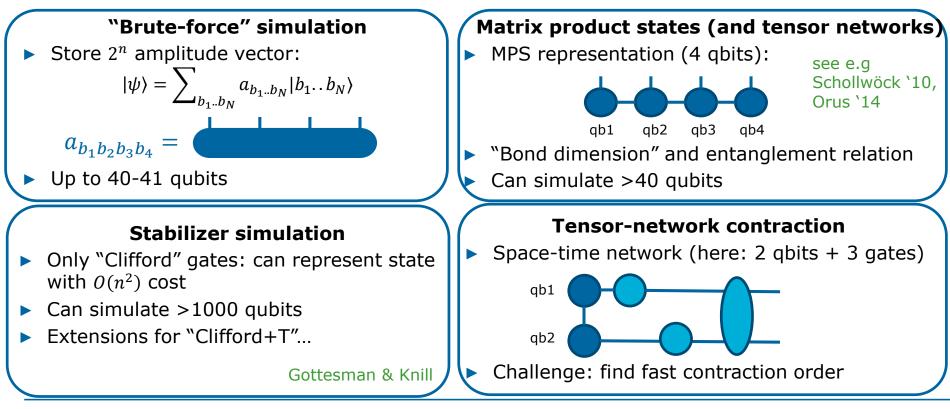
Simulation:

$$\rho_f = \mathcal{E}_M \circ \cdots \circ \mathcal{E}_1(\rho_i)$$



Ideal circuit simulation

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



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Noisy simulation

Density-matrix evolution:

Use e.g 'Kraus' representation

 $\rho_f = \sum_{k_M} \left(E_{k_M}^{(M)} \dots \left(\sum_{k_1} E_{k_1}^{(1)} \rho E_{k_1}^{(1)\dagger} \right) \dots E_{k_M}^{(M)\dagger} \right)
 ~OK for <20 qubits$

Stochastic sampling:

- Can use ideal circuit simulator to compute each "trajectory" $|\psi_i\rangle$
- Can simulate many more qubits

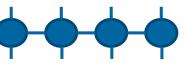
Near-Clifford simulation

- Decompose $\mathcal{E}^{(j)} = \sum_i q_i^{(j)} S_i$ with S_i stabilizer channel
- Sample resulting sum over stabilizer channels

Bennink et al

Matrix product operators (and tensor networks)

MPO representation (4 qbits):





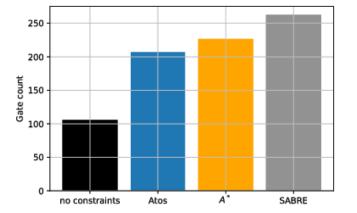


Optimization

developing quantum programs in a hardwareagnostic way... but suitably optimized for a target platform

Example 1: Compilation of a Quantum Fourier Transform

- Fourier transform on IBM's 14-qbit Melbourne chip Need to insert SWAPs + use only CNOTs
- Two different optimization metrics:

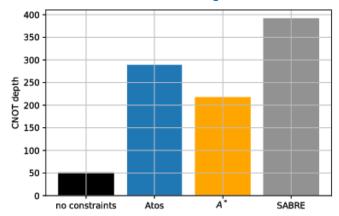


Gate count

Connectivity map:



CNOT depth



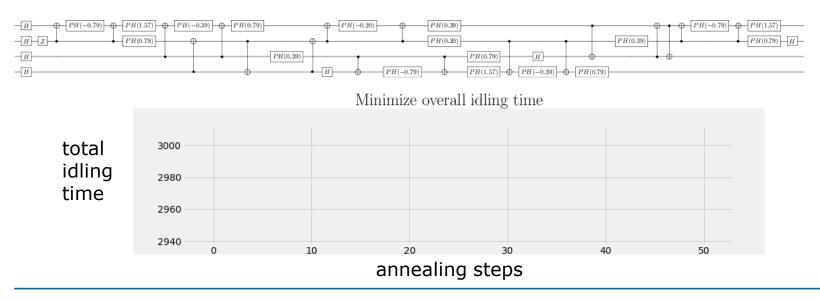
*A**: 1712.04722, SABRE: 1809.02573

1 SWAP=3 CNOTs, 1 C-PH=2 CNOTs



Example 2: Minimization of the total idling time

- Start compiled Quantum Fourier (here 4 qubits)
- Use commutation patterns to reduce total idling time
- Minimization via (classical) simulated annealing

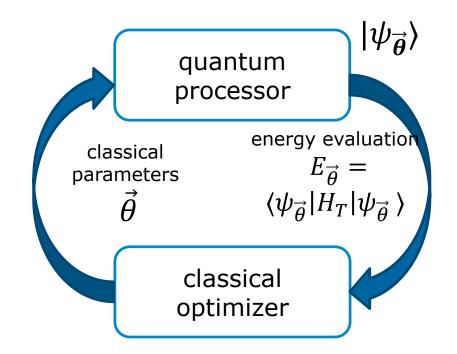






Variational quantum algorithms

- Overcome
 - short coherence times
- Split work between
 - quantum processor
 - classical optimizer
- Goal:
 - find lowest eigenenergy of Hamiltonian H_T





Applications of variational quantum algorithms

- Quantum chemistry ("VQE")
 - Many small molecules (H2, LiH, ...)
 - Well-known variational states: unitary coupled cluster (UCC), etc.
- Combinatorial optimization ("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:

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

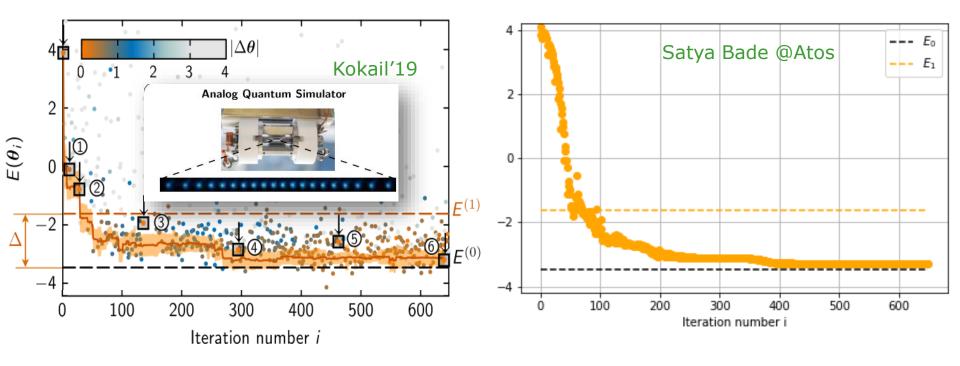
with mass m, coupling g



Challenge II: Experimental realization and simulation

Experimental result (Nions=8):

Our simulation (Nions=8)

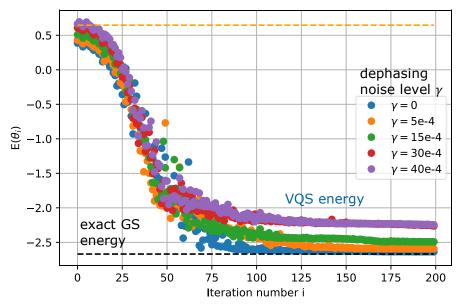


See also: digital computation with 4 ions (Martinez et al, Nature '16), 5 SC qubits (Klco et al PRA '18), ...



Going beyond: impact of noise

- Noisy simulations with varying noise levels
 - Dephasing noise (Lindblad equation)







Demonstration

A Noisy Quantum Fourier Transform on the Atos Quantum Learning Machine

- Key ingredient of quantum factoring algorithms ("Shor algorithm")
- From time to frequency: Fourier Signal 0.6 0.06 0.5 spectrum 0.05 0.4 0.04 0.3 0.03 0.2 0.02 0.01 0.0 10

 $P = 32 = 2^5$ time points

- Best known classical algorithm: Fast Fourier Transform Number of operations: ~ $P \log P$ for a signal of size P
- Quantum Fourier Transform (QFT):

log P log P operations: exponential speedup!

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A Noisy Quantum Fourier Transform on the Atos Quantum Learning Machine

Demonstration: simulate a (noisy) processor on the QLM



Part I: Writing an universal quantum program

Part II: IBM QX4 - superconducting qubits

Part III: AQTion-related results - trapped ions

Part I: Writing an universal quantum program

Example: Quantum Fourier transform, $QFT(|x\rangle) = \frac{1}{\sqrt{2^n}} \sum_{k=0}^{2^n-1} \left(e^{\frac{2i\pi}{2^n}}\right)^{k} |k\rangle$

Key ingredient to e.g Shor's factoring algorithm.

I.1 Writing the quantum program

The QLM provides usual quantum gates + libraries of quantum routines

```
Entrée [1]: from qat.lang.AQASM import Program
from qat.lang.AQASM.qftarith import QFT
from qat.linalg.oracles import StatePreparation
from demo_init import prepare_ft_signal, format_qft_output
nqbits = 5
prog = Program()
reg = prog.qalloc(nqbits)
state_prep = StatePreparation(prepare_ft_signal(nqbits))
prog.apply(state_prep, reg)
prog.apply(QFT(nqbits), reg)
qft_circ_boxed = prog.to_circ(inline=False)
```

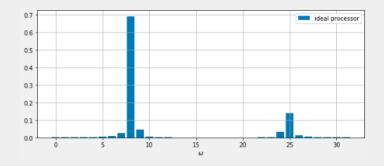
```
%qatdisplay qft_circ_boxed
```



I.2 Ideal simulation

```
Entrée [2]: import numpy as np
import matplotlib.pyplot as plt
%pylab inline
from qat.qpus import LinAlg
results = LinAlg().submit(qft_circ_boxed.to_job())
resprobs = np.zeros(shape=(2**nqbits))
for result in results.raw_data: resprobs[result.state.int]=result.probability
plt.figure(figsize=(10,4))
plt.bar(np.array(range(2**nqbits)), np.abs(format_qft_output(resprobs)), width=4/5, label="ideal processor")
plt.legend(); plt.grid(); plt.xlabel(r"$\omega$");
```

Populating the interactive namespace from numpy and matplotlib

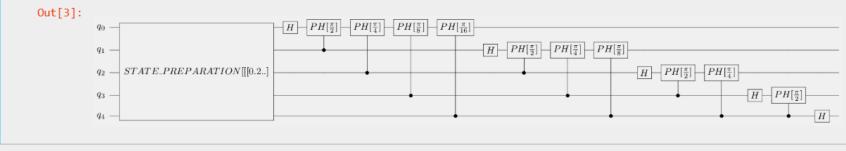


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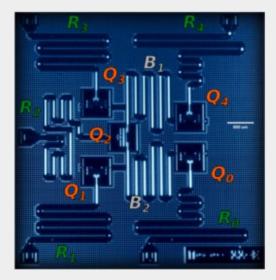
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I.3 Universal circuit

Entrée [3]: qft_circ = prog.to_circ(inline=True)
print("Number of gates:", len(qft_circ))
%qatdisplay qft_circ
Number of gates: 16

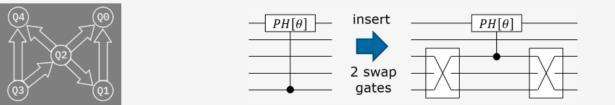


Part II: IBM QX4 - superconducting qubits



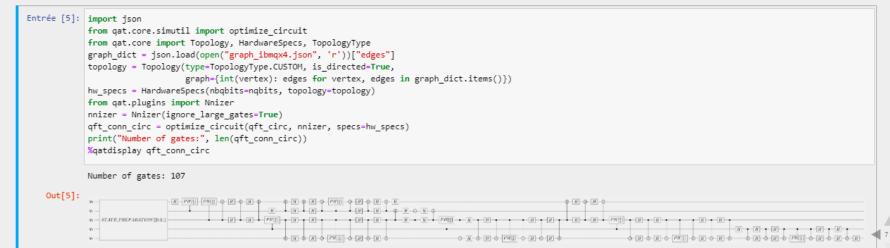
II.1 Connectivity

IBM QX4 has a limited qubit connectivity:



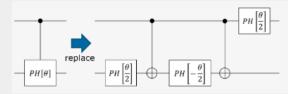
Entrée [4]: %cat graph_ibmqx4.json

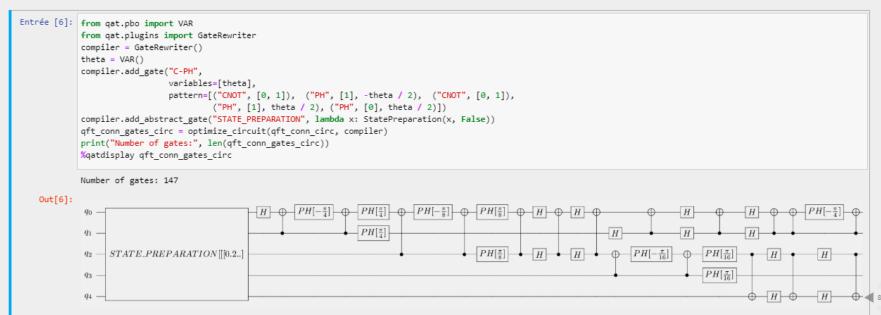
{"edges": {"1": [0], "2": [0, 1, 4], "3": [2, 4]}}



II.2 Compilation (continued)

IBM QX4 only accepts CNOT gates for two-qubit operations:

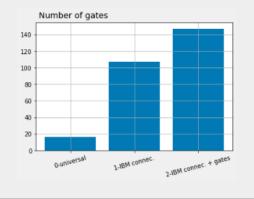




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II.3 Gate counts before and after compilation

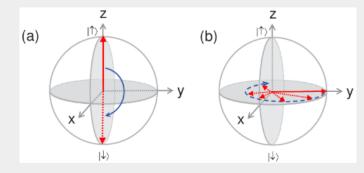




II.4 Noisy simulation

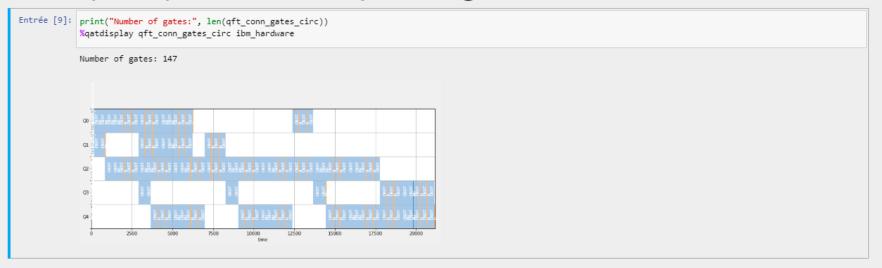
Live simulation of noisy simulation on Atos QLM, with **simplified hardware model**:

- "Idle" qubits suffer from decoherence: **amplitude damping** (A.D) and **pure dephasing** (P.D).
- Relaxation and dephasing times from constructor: T_1 and T_2



Entrée [8]:	from qat.hardware import DefaultGatesSpecification, HardwareModel
	<pre>from qat.core.circuit_builder.matrix_util import get_predef_generator</pre>
	<pre>from qat.quops.quantum_channels import ParametricPureDephasing, ParametricAmplitudeDamping</pre>
	gate_durations = {"H":60, "X":120, "Y":120, "S":1,"T":1, "D-T":1, "Z":1,
	"RZ": lambda angle: 1, "PH": lambda angle: 1, "C-PH": lambda angle: 1,
	"CNOT":386, "SWAP" :100, "STATE_PREPARATION": 10}
	<pre>pred_generator = get_predef_generator()</pre>
	<pre>pred_generator["STATE_PREPARATION"] = prepare_ft_signal(nqbits)</pre>
	<pre>ibm_gates_spec = DefaultGatesSpecification(gate_durations, predef_generator=pred_generator)</pre>
	T1, T2 = 44000, 38900 #nanosecs
	$amp_damping = ParametricAmplitudeDamping(T_1=T1)$
	<pre>pure_dephasing = ParametricPureDephasing(T_phi=1/(1/T2 - 1/(2*T1)))</pre>
	<pre>ibm_hardware = HardwareModel(ibm_gates_spec, idle_noise=[amp_damping, pure_dephasing])</pre>

II.5 Temporal representation of the quantum algorithm

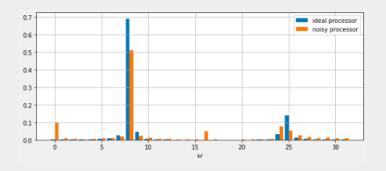


11.1

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II.6 Result: Noisy Fourier spectrum

Entrée [10]: import numpy as np
from qat.qpus import LinAlg, NoisyQProc
from qat.plugins import QuameleonPlugin
plt.figure(figsize=(10,4))
ideal_qpu = LinAlg()
noisy_qpu = nnizer | compiler | QuameleonPlugin(specs=hw_specs) | NoisyQProc(hardware_model=ibm_hardware)
for nqpu, (qpu, label) in enumerate([(ideal_qpu, "ideal processor"), (noisy_qpu, "noisy processor")]):
 results = qpu.submit(qft_circ.to_job())
 allprobs = np.zeros(shape=(2**nqbits))
 for result in results.raw_data: allprobs[result.state.int]=result.probability
 plt.bar(np.array(range(2**nqbits))+nqpu*2/5-1/5, np.abs(format_qft_output(allprobs)), width=2/5, label=label)
plt.legend(); plt.grid(); plt.xlabel(r"\$\omega\$");



II.7 Fidelity optimization

st - STATE PREPARATION [0.2.] -

 $-PH[\frac{1}{20}]$

PHILIN PHILIN

```
Entrée [11]: from gat.plugins import PatternManager
             from qat.noisy.noisy circuit import total idling time
             metric = lambda circ: -total idling time(circ, ibm hardware)
             manager = PatternManager(global metric=metric)
             x, y = VAR(), VAR()
             group1 = manager.new group()
             group1.add_pattern([('PH', [1], x), ('CNOT', [0, 1]), ('PH', [1], y), ('CNOT', [0, 1])])
             group1.add pattern([('CNOT', [0, 1]), ('PH', [1], y), ('CNOT', [0, 1]), ('PH', [1], x)])
             group2 = manager.new group()
             group2.add pattern([('PH', [1], x), ('CNOT', [0, 1]), ('H', [0]), ('H', [1]), ('CNOT', [0, 1]), ('H', [0]), ('H', [1]), ('CNOT', [0, 1])])
             group2.add pattern([('CNOT', [0, 1]), ('H', [0]), ('H', [1]), ('CNOT', [0, 1]), ('H', [0]), ('H', [1]), ('CNOT', [0, 1]), ('PH', [0], x)])
             group3 = manager.new group()
             group3.add pattern([('PH', [0], x), ('CNOT', [0, 1]), ('H', [0]), ('H', [1]), ('CNOT', [0, 1]), ('H', [0]), ('H', [1]), ('CNOT', [0, 1])])
             group3.add pattern([('CNOT', [0, 1]), ('H', [0]), ('H', [1]), ('CNOT', [0, 1]), ('H', [0]), ('H', [1]), ('CNOT', [0, 1]), ('PH', [1], x)])
             group4 = manager.new group()
             group4.add_pattern([('PH', [1], x), ("H", [1]), ("CNOT", [0, 1]), ("H", [1])])
             group4.add_pattern([("H", [1]), ("CNOT", [0, 1]), ("H", [1]), ('PH', [1], x)])
             group5 = manager.new group()
             group5.pattern_to_remove([('PH', [0], x), ('PH', [0], y)])
             group5.add_pattern([('PH', [0], x + y)])
             group6 = manager.new_group()
             group6.pattern to_remove([('CNOT', [0, 1]), ('CNOT', [0, 1])])
             group6.pattern to remove([('H', [0]), ('H', [0])])
             group6.add pattern([])
             manager.add abstract gate("STATE PREPARATION", lambda x: StatePreparation(x, False))
             qft fid optim circ = manager.replace pattern(
                 qft conn gates circ, method="annealing", max iterations=250)
             print("Number of gates:", len(qft fid optim circ))
             %qatdisplay qft fid optim circ
             Number of gates: 79
   Out[11]:
                                                                                                                                   H + H + PH
```

⊕ PH[-5] ⊕ PH[127]

PH[-[] - PH[-]] - H

28141

PH [-]_

R

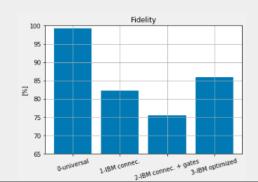
- R - PH[0.15] - PH[-1,1] - O

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II.8 Results

```
Entrée [12]: from qat.noisy import compute_fidelity
print("Initial idle time:", total_idling_time(qft_conn_gates_circ, ibm_hardware))
print("Final idle time:", total_idling_time(qft_fid_optim_circ, ibm_hardware))
fid_1 = compute_fidelity(qft_circ, ibm_hardware, use_linalg=True)
fid_2 = compute_fidelity(qft_conn_circ, ibm_hardware, use_linalg=False)
fid_3 = compute_fidelity(qft_conn_gates_circ, ibm_hardware, use_linalg=False)
fid_4 = compute_fidelity(qft_fid_optim_circ, ibm_hardware, use_linalg=False)
plt.bar(["0-universal", "1-IBM connec.", "2-IBM connec. + gates", "3-IBM optimized"],
        [fid_1[0]*100, fid_2[0]*100, fid_3[0]*100, fid_4[0]*100])
plt.title("Fidelity"); plt.xticks(rotation=15); plt.ylim(65,100); plt.grid();
plt.ylabel("[%]");
```

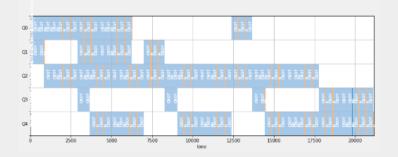
Initial idle time: 56722 Final idle time: 28106

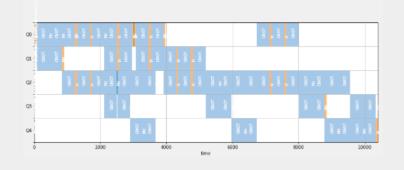


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Entrée [13]: print("Number of gates:", len(qft_conn_gates_circ))
%qatdisplay qft_conn_gates_circ ibm_hardware
print("Number of gates:", len(qft_fid_optim_circ))
%qatdisplay qft_fid_optim_circ ibm_hardware

Number of gates: 147 Number of gates: 79





 \mathbf{eta}

15.1

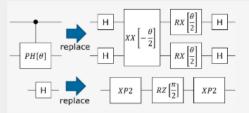
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Part III: AQTion-related results - trapped ions



III.1 Compiling for ions

We use the same plugin as for IBM, but with different patterns:



Use abstract gates to create custom parametrized gates, like

$$XX[\phi] = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & -ie^{i\phi} \\ 0 & 1 & -i & 0 \\ 0 & -i & 1 & 0 \\ -ie^{-i\phi} & 0 & 0 & 1 \end{bmatrix}$$

```
Entrée [14]: from gat.pbo import VAR
              from qat.plugins import GateRewriter
              gr compiler = GateRewriter()
              theta = VAR()
              ## C-PH => XX & H & R7
              gr compiler.add gate("C-PH",
                                      variables=[theta],
                                      pattern=[("H", [0]), ("H", [1]), ("XX", [0, 1], -theta/2),
                                               ("RX", [0], theta/2), ("RX", [1], theta/2), ("H", [0]), ("H", [1])])
              ## H => XZX
              gr_compiler.add_gate("H",
                                 variables=[],
                                 pattern=[("XP2", [0]), ("RZ", [0], np.pi/2), ("XP2", [0])])
              ## RX(theta) ==> XP2 & RZ(theta)
              gr_compiler.add_gate("RX",
                                      variables=[theta],
                                      pattern=[("RZ", [0], np.pi/2), ("XP2", [0]), ("RZ", [0], theta - np.pi),
                                               ("XP2", [0]), ("RZ", [0], np.pi/2)])
              gr compiler.add abstract gate("STATE PREPARATION", lambda x: StatePreparation(x, False))
              from ion gate set import ion gate set
              for , gatedef in ion gate set.gate signatures.items():
                  gr compiler.add abstract gate(gatedef)
              qft gates circ = optimize circuit(qft circ, gr compiler | gr compiler)
              print("Number of gates:", len(qft gates circ))
              %qatdisplay qft gates circ
              Number of gates: 246
   Out[14]:
                                                           RZ[\frac{\pi}{2}]
                                                                     XP2 - XP2 - RZ[\frac{\pi}{2}] - XP2 -
                                                                                                              RZ[\frac{\pi}{2}] XP2 RZ[-2.36]
                                                                                                                                         -XP2 -RZ[\frac{\pi}{2}] -XP2 -RZ[\frac{\pi}{2}] -XP2 -XP2 -h
               q_0
                                                     XP2
                                                                                                    XX[-\frac{\pi}{4}]
                                                    XP2 - RZ[\frac{\pi}{2}] - XP2
                                                                                                               RZ[\frac{\pi}{2}] XP2 RZ[-2.36] XP2 RZ[\frac{\pi}{2}] XP2 RZ[\frac{\pi}{2}] XP2
               q_1
                   STATE_PREPARATION[[[0.2..]
                                                   XP2 - RZ[\frac{\pi}{2}]
                                                                    -XP2
               q_2 =
                                                    XP2 - RZ[\frac{\pi}{2}]
                                                                    XP2
               q_3
```

 $XP2 \longrightarrow RZ[\frac{\pi}{2}] \longrightarrow XP2$

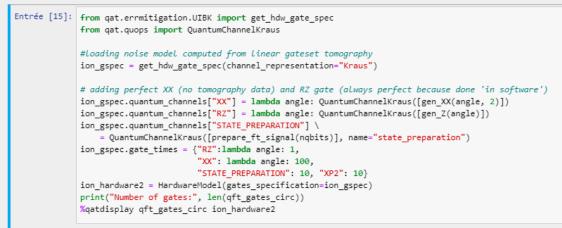
18.1

?

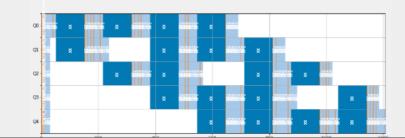
 $q_4 =$

III.2 Noisy simulation with tomography data

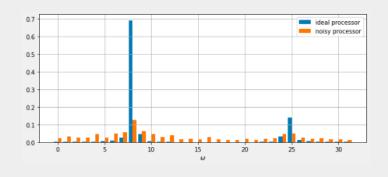
Here we load a noise model computed by performing tomography of some gates of the trapped-ion processor of the University of Innsbruck (UIBK):



Number of gates: 246



```
Entrée [16]: from ion_gate_set import gen_X, gen_Z, gen_XX
compiler = gr_compiler | gr_compiler #need 2 passes to replace all patterns
ideal_qpu = LinAlg()
noisy_qpu = compiler | NoisyQProc(hardware_model=ion_hardware2)
plt.figure(figsize=(10,4))
for nqpu, (qpu, label) in enumerate([(ideal_qpu, "ideal processor"), (noisy_qpu, "noisy processor")]):
    results = qpu.submit(qft_circ.to_job())
    allprobs = np.zeros(shape=(2**nqbits))
    for result in results.raw_data: allprobs[result.state.int]=result.probability
    plt.bar(np.array(range(2**nqbits))+nqpu*2/5-1/5, np.abs(format_qft_output(allprobs)), width=2/5, label=label)
plt.legend(); plt.grid(); plt.xlabel(r"$\omega$");
```



In summary,

We have

 \Rightarrow defined a simple universal circuit

with an Oracle and a QRoutine from the QLib

 \Rightarrow simulated it on a perfect QPU

with the ideal Linear Algebra simulator

 \Rightarrow optimized it for specific hardware (superconducting qubits and trapped ions)

with NNizer (for topology),

with Pattern-Based Optimizer (for gate replacement and idle time optimization)

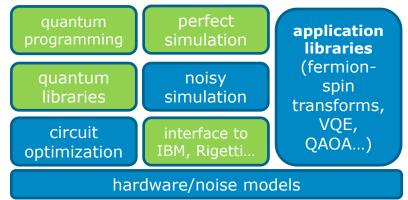
with Abstract Gates

with Noise Simulation

Conclusion

- Hands-on tutorial this afternoon (3:30pm) with Jean-Christophe Jaskula
 - make sure you have downloaded the myQLM docker
- Menu:
 - write and run quantum programs
 - varational minimization using quantum circuits

myQLM: "QLM lite", free!





Thank you

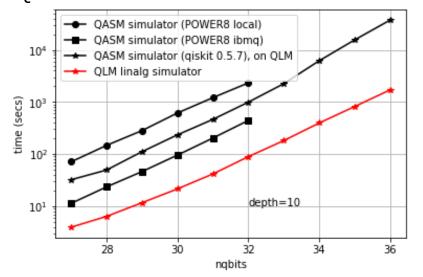
thomas.ayral@atos.net

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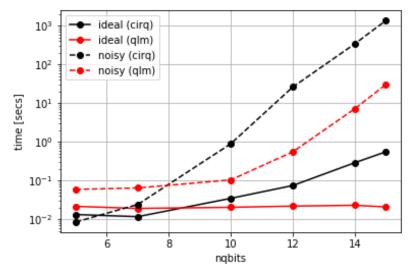


Speed comparison

QLM vs IBM Qiskit simulator Perfect simulation 'Quantum volume' benchmark circuit



QLM: **qat.linalg** simulator IBM POWER8 benchmark data from www.ibm.com/blogs/research/2018/05/quantum-circuits QLM vs Google cirq simulator Perfect + noisy simulation H+CNOT circuit



QLM: qat.linalg and qat.noisy (deterministic-vectorized) simulator

