Practical QC School 22

Combinatorial Optimization, Variational algorithms and QAOA through Atos's environment

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01/12/2022

Today's agenda

01. A dive into the Atos Quantum Program

02. Combinatorial Optimization, Variational algorithms and their Quantum Applications

03. QAOA and Max-Cut, simulation through a QLM

01.

A dive into the Atos Quantum Program

Who we are and what we do

Atos

European at heart

- Founded in 1997, started in France, quickly became a global reality
- With 150.000+ employees
- Billing more than 11 billions yearly and investing 235m in R&D
- We deliver In 71 countries all across the globe

Atos Worldwide IT Partner

Atos Italia

Excellence & Acceleration

- Founded in 2011, focusing on innovation and development of the country
- With 1500+ employees in 5 locations
- Billing more than 300 millions yearly
- Organized in 6 industries to ensure excellence for our customers

Manufacturing

Resources, Utilities Transport & Logistics

Financial & insurance

Telecom, Media & Technology

Public sector & defence

Healthcare & lifestyle

Our customers

FCA FIAT CHRYSLER AUTOMOBILES
LEONARDO
Mercedes-Benz
PIAGGIO
FINCANTIERI

vodafone
FASTWEB
Disney
open fiber

EDF
eni
a2a
TOTAL

CINECA
MINISTERO DELLA DIFESA
EUROPEAN COMMISSION
DIRECTORATE-GENERAL
Joint Research Centre
INPS

GENERALI
UniCredit
BNL
GRUPPO BNP PARIBAS

BAYER
Epic
SIEMENS Healthineers

Atos
Worldwide IT Partner

Big Data and Security – BDS Italy

We build realities with our clients

High Performance Computing

Fourth most powerful HPC with Leonardo CINECA

Leonardo Finmeccanica Da Vinci's cluster

Quantum Computing

Q@TN with UniTrento and FBK

PQCS CINECA

Cybersecurity

ENI SAP management

Fastweb Law Enforcement Architecture

Artificial Intelligence

Automation and efficiency with Generali

Computer Vision

Atos Worldwide IT Partner

Leader in decarbonization

Improving energy efficiency and carbon emissions

Reducing carbon emissions by 50% by 2025, offsetting by 2028

Choosing hardware that ensure energy saving

Helping companies deal with sustainability challanges

Atos's plan

Simulations to simplify real problems

"Let's look at Quantum Computers as accelerators, not as independent systems"

- Hardware agnostic
- Simulators for an experimental approach
- Based on our HPC and simulations experience
- "All inclusive"
- Open platform

Atos's Quantum Roadmap approach

- **2016** – Launch of Quantum program
- **2017** – Release and installation of the first QLM
- **2018** – Noisy simulations
- **2019** – myQLM & QLM user club
- **2020** – Simulated Annealing
- **2023+** – QPU offering

The Quantum Program in 5 steps

Quantum Programming Platform

Quantum Expert Consulting Services

Quantum Algorithms

New Generation Architecture

Quantum Safe Cryptography

The Atos Quantum Program

Empowering international research on Quantum Computing

Quantum applications	Quantum algorithms	Next-generation architectures
<NE|AS|QC>	QUANTERA	AQTION
Université de Lorraine	IRIF Institut de Recherche en Informatique Fondamentale	PASQuanS
HQS	ANR Agence Nationale de la Recherche	IQM
AstraZeneca	université PARIS-SACLAY	AQT
Universiteit Leiden	CentraleSupélec	PASQAL
eDF		
ICHEC Irish Centre for High-End Computing		
HSBC		
CESGA Centro de Supercomputación de Galicia		
TotalEnergies		

A choice made by many

Thanks to our openness and scalability, we work with scientific communities, companies and universities to bring the future a step closer

The Atos QLM: our appliance

The result of our commitment

Built to face real problems, now

Designed to interface with real QPUs

Universal programming environment

myQLM

The entry level of our Quantum offering

Freeware desktop solution

Entry level simulation

Scalability ~20 qubits

Q-score

The new quantum LINPACK

A new quantum metrics reference, applicable to **all** quantum circuits

Measures the efficiency to run a representative quantum application, instead of pure technical KPIs

Offering universal and free access to Q-score

What does it offer?

A complete programming environment

Programming

AQASM
Assembly language to build quantum circuits

pyAQASM
Python extension to AQASM

CIRC
Binary format of quantum circuits

QLIB
AQASM & pyAQASM libraries

CO problems class
Describe any Combinatorial Optimization problem

INTEROP
Connectors with other frameworks

ProjectQ

Qiskit

Optimization

PBO
Pattern based optimizer

NNIZER
Topology constraint solver

Circuit Optimizer
Generic circuit optimizer

Simulation

Simulators
Digital QC Simulators
Quantum-Inspired Simulators

Physics
Physical Noise models

What does it offer?
Interoperability with python based frameworks

- Providing binders to translate Quantum circuits
- Back and fourth from QLM to QPUs and simulators

What are the possible ways to use the Atos QLM?

A multi-purpose system

Learn

Get acquainted with quantum computing

Test

Conceive new programs and debug them

Optimize

Select the best quantum technology to solve your problem

Run hybrid code

Off-load the quantum-accelerable parts to the simulated QPU

Électricité de France

QC in Energy Utilities

Optimal battery operation

Batteries on a national scale for renewables energy

Smart charging for electric vehicles

Positioning of load-station on a wide-range map

Probabilistic Risk and Safety assessment

Probability estimation and application of optimal strategies

BMW Group
QC in manufacturing

Process scheduling
Optimization of major shops to maximize throughput

Quantum Circuits for ML training
Faster and optimal Computer vision for inspections

Optimal order of production
Lower the production cost with best quality and lowest rework

BMW GROUP

Total Energies

QC in Oil&Gas Industry

Solving complex partial differential equations

Different applications in many camps of interest

Tackling decarbonization

Simulation of large complex molecules for efficient adsorbents

Supporters of the Atos Quantum Approach

Co-chair of the Atos QLM User Club

TotalEnergies

Atos QLM

Enabling research since 2017

Reuse method for quantum circuit synthesis – *AMMCS 2017*
C. Allouche, M. Baboulin, T. Goubault de Brugière, and B. Valiron

Electron-Phonon Systems on a Universal Quantum Computer – *Phys Rev Lett 2018*
A. Macridin, P. Spentzouris, J. Amundson, and R. Harnik

Digital quantum computation of fermion-boson interacting systems – *Phys Rev A 2018*
A. Macridin, P. Spentzouris, J. Amundson, and R. Harnik

Synthesizing Quantum Circuits via Numerical Optimization – *ICCS 2019*
T. Goubault de Brugière, M. Baboulin, B. Valiron, and C. Allouche

q-means: A quantum algorithm for unsupervised machine learning – *NIPS 2019*
I. Kerenidis, J. Landman, A. Luongo, and A. Prakash

Function Maximization with Dynamic Quantum Search – *QTOP 2019*
C. Moussa, H. Calandra, and T. S. Humble

Methods for Classically Simulating Noisy Networked Quantum Architectures – *QST 2019*
I. Vankov, D. Mills, P. Wallden, and E. Kashefi

Practical implementation of a quantum backtracking algorithm – *Sofsem 2020*
S. Martiel, M. Remaud

Atos QLM

Enabling research since 2017

Quantum CNOT Circuits Synthesis for NISQ Architectures Using the Syndrome Decoding Problem – *Rev Comp 2020*
T. G. de Brugière, M. Baboulin, B. Valiron, S. Martiel, and C. Allouche

Quantum circuits synthesis using Householder transformations – *CPC 2020*
T. Goubault de Brugière, M. Baboulin, B. Valiron, and C. Allouche

Classification of the MNIST data set with quantum slow feature analysis – *Phys Rev A 2020*
I. Kerenidis and A. Luongo

Quantum Divide and Compute: Hardware Demonstrations and Noisy Simulations – *IVLSI 2020*
T. Ayral, F.-M. L. Régent, Z. Saleem, Y. Alexeev, and M. Suchara

To quantum or not to quantum: towards algorithm selection in near-term quantum optimization – *QST 2020*
C. Moussa, H. Calandra, and V. Dunjko

Arrays vs. Decision Diagrams: A Case Study on Quantum Circuit Simulators – *ISMVL 2020*
T. Grurl, J. Fuß, S. Hillmich, L. Burgholzer, and R. Wille

Considering decoherence errors in the simulation of quantum circuits using decision diagrams – *ICCAD39 2020*
T. Grurl, J. Fuß, and R. Wille

Solving optimization problems with Rydberg analog quantum computers: Realistic requirements for quantum advantage using noisy simulation and classical benchmarks – *Phy Rev A 2020*
M. F. Serret, B. Marchand, and T. Ayral

Atos QLM

Enabling research since 2017

Stochastic Quantum Circuit Simulation Using Decision Diagrams – *arXiv 2020*
T. Grurl, R. Kueng, J. Fuß, and R. Wille

Qualifying quantum approaches for hard industrial optimization problems. A case study in the field of smart-charging of electric vehicles – *arXiv 2020*
C. Dalyac et al.

Practical Quantum Computing: Solving the Wave Equation Using a Quantum Approach – *ACM Transactions on QC 2021*
A. Suau, G. Staffelbach, and H. Calandra

Benchmarking quantum co-processors in an application-centric, hardware-agnostic and scalable way – *arXiv 2021*
S. Martiel, T. Ayral, and C. Allouche

Quantum Divide and Compute: Exploring the Effect of Different Noise Sources – *SN COMPUT. SCI. 2021*
T. Ayral, F.-M. L. Régent, Z. Saleem, Y. Alexeev, and M. Suchara

Quantum Computing: Towards Industry Reference Problems – *Digitale Welt 2021*
A. Luckow, J. Klepsch, and J. Pichlmeier

myQLM

Click on the picture or visit
myqlm.github.io

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02.

Combinatorial Optimization and Variational Algorithms

A first approach and applications in the Quantum Realm

Combinatorial Optimization

What are we talking about?

Operations Research

- Deals with development and application of analytical methods, to improve decision-making
- Employing techniques such as modeling, statistics and optimization
- Emphasis on practical applications

Optimization problems

- Find the best solution among many others
- Applied on real world scenarios but as mathematical models
- Algorithmic approach to solutions
- Becomes combinatorial when such variables are discrete

Combinatorial optimization
Applications

- Industrial problems
  - Production planning
  - Localization of facilities
  - Stock management
- Organization problems
  - Routing
  - Scheduling of work shifts
  - Management of water resources
- Optimal planning
  - Network planning
  - Structures planning
  - VLSI design
- Economics decision-making problems
  - Capitals allocation
  - Purchase/Sell of products
  - Choose investment

Combinatorial optimization

Modelling approach

1. Analysis of the problem
2. Construction of the model
3. Analysis of the model
4. Numeric solution
5. Validation of the problem

Combinatorial optimization

Structure of decision-making problems

Objective

Decision-making variables

Constraints

Mathematical model

Combinatorial optimization

Example of a mathematical model

- A company sells 3 types of cars: suv, convertible and minivan
- They use 2 type of production machines, M1 and M2.
- To make a suv, they need 4 hours on M1 and 3 on M2; for a convertible they need 8 hours on M2 and for a minivan they need 2 hours on M1 and 5 on M2.
  M1 is avaiable for 120 hours a week, while M2 is avaiable for 90 hours a week.
- The company wants to produce at least 3 convertible a week
- They sell a suv for 1200€, a convertible for 1500€ and a minivan for 1800€
- And then, they ask us to gain as much as possible from this production system.

Objective

- Maximize profit

Variables

- Suv, convertible, minivan
- M1, M2

Constraints

- M1 for 120 hours
- M2 for 90 hours
- At least 3 convertibles

Combinatorial optimization

Example of mathematical model

Objective

- Maximize profit

Maximization function

$$maz\ Z = 1200x_1 + 1500x_2 + 1800x_3$$

Variables

- Suv, convertible, minivan
  - M1, M2

$$x_1, x_2, x_3\ ;\ M_1, M_2$$

$$x_1, x_2, x_3\ \geq 0$$

Constraints

- M1 for 120 hours
- M2 for 90 hours
  - At least 3 convertibles

$$\Sigma M1\ \leq 120;$$
$$\Sigma M2\ \leq 90;$$
$$x_2 \geq 3$$

$$4x_1 + 2x_3\ \leq 120$$
$$3x_1 + 8x_2 + 5x_3\ \leq 90$$
$$x_2\ \geq 3$$

Combinatorial optimization

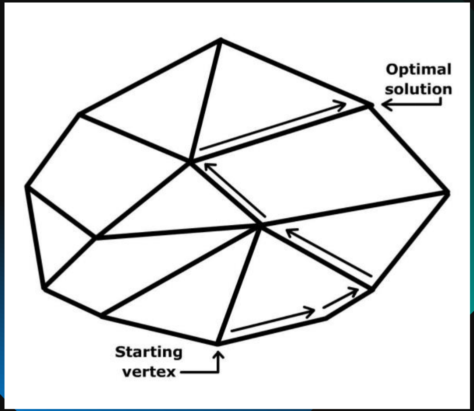
Example of mathematical model

$$\begin{aligned}
max\ Z = 1200x_1 + 1500x_2 + 1800x_3 \\
4x_1 + \qquad\qquad 2x_3 \leq 120 \\
3x_1 + \quad 8x_2 + \quad 5x_3 \leq 90 \\
x_2 \qquad\qquad \geq 3 \\
x_1, \quad x_2, \quad x_3 \geq 0
\end{aligned}$$

Combinatorial optimization

The Simplex and why we are searching for new algorithms

- Used to resolve linear programming problems
- Utilizes a polytope to optimize problems
- Find solutions in the corners
- Widely used even if polynomial in worst case scenario



Combinatorial optimization

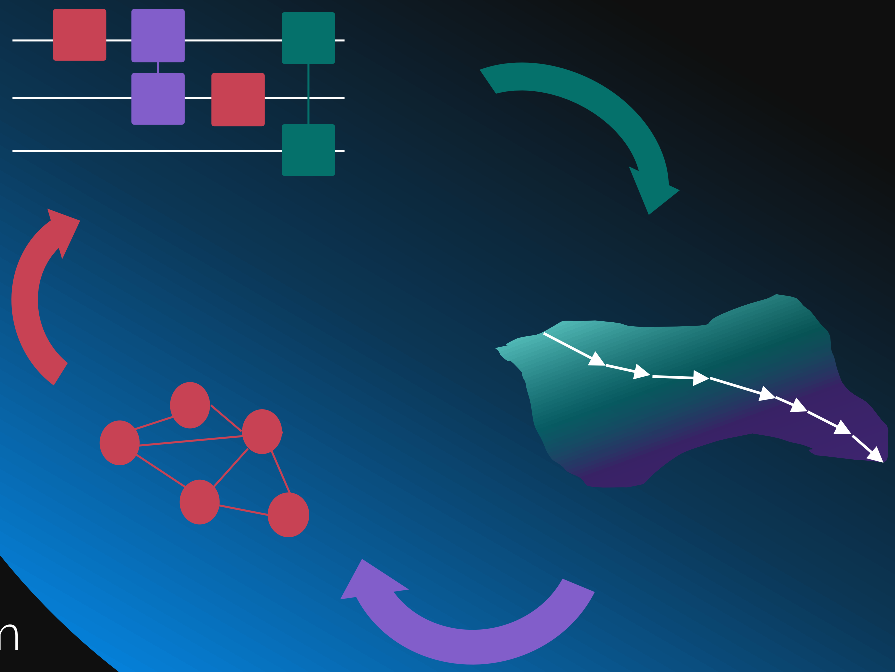
Solutions landscape, how many people to change a lightbulb?

- There are multiple algorithms and methods for CO and OR
- Sometimes even for the same problem

- A lot of problems require gargantuan calculus
- Approximation for heuristic solutions

Variational algorithms
Quantum evolution

- Encode the problem in the energy landscape
- Find a trial lowest energy point
- Exclude points from landscape
- Iterate until you find the global minimum

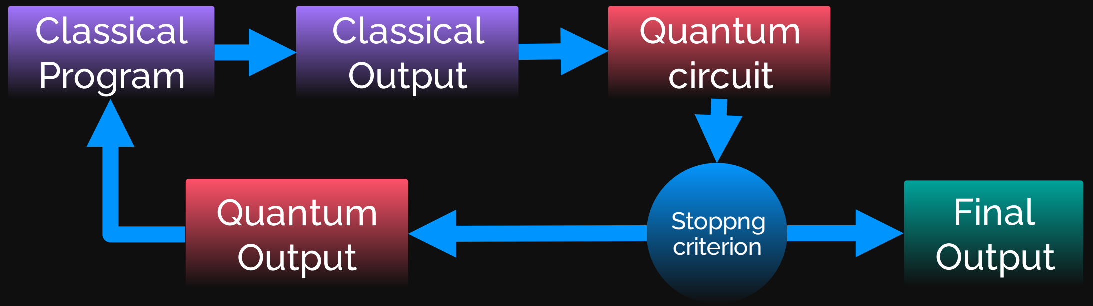


Variational algorithms

A NISQ optimization routine

A working application for the current NISQ systems

- Classical optimizer to leverage on quantum properties
- Loop feedback



Variational algorithms
Some examples

- VQE
- VITE
- VQF

- Chemistry related, finds the ground state
- Another promising way to find ground states
- Breakdown factoring in a NISQ system

Quantum Approximate Optimization Algorithm
Formulating combinatorial problems

Our problems can be formulated as a cost function

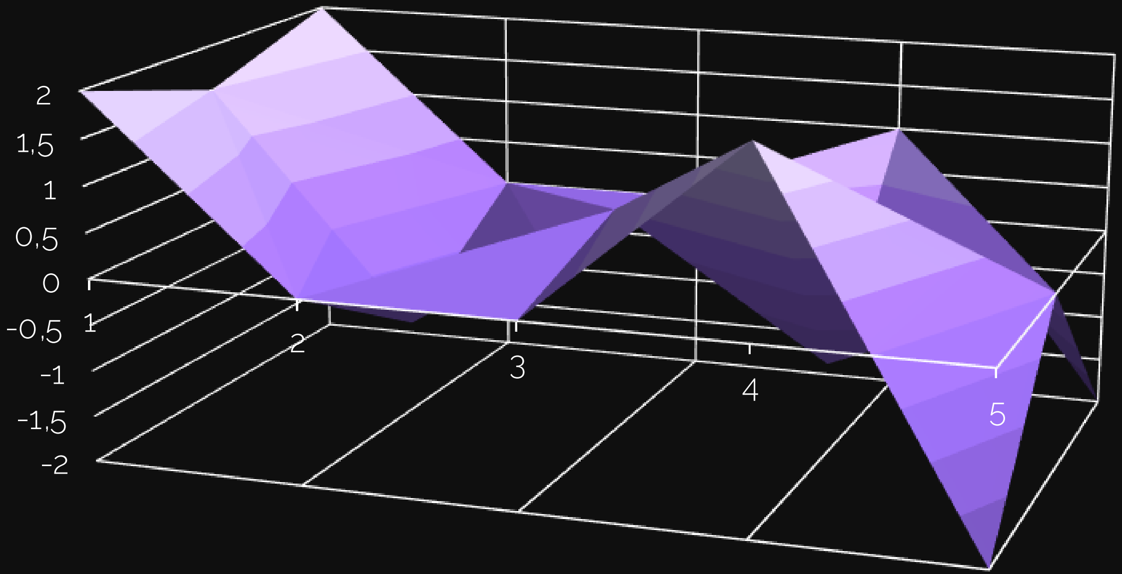
Finding the ground state, is a minimization problem

We use this similarity to resolve QUBO and Ising problems

Quantum Approximate Optimization Algorithm

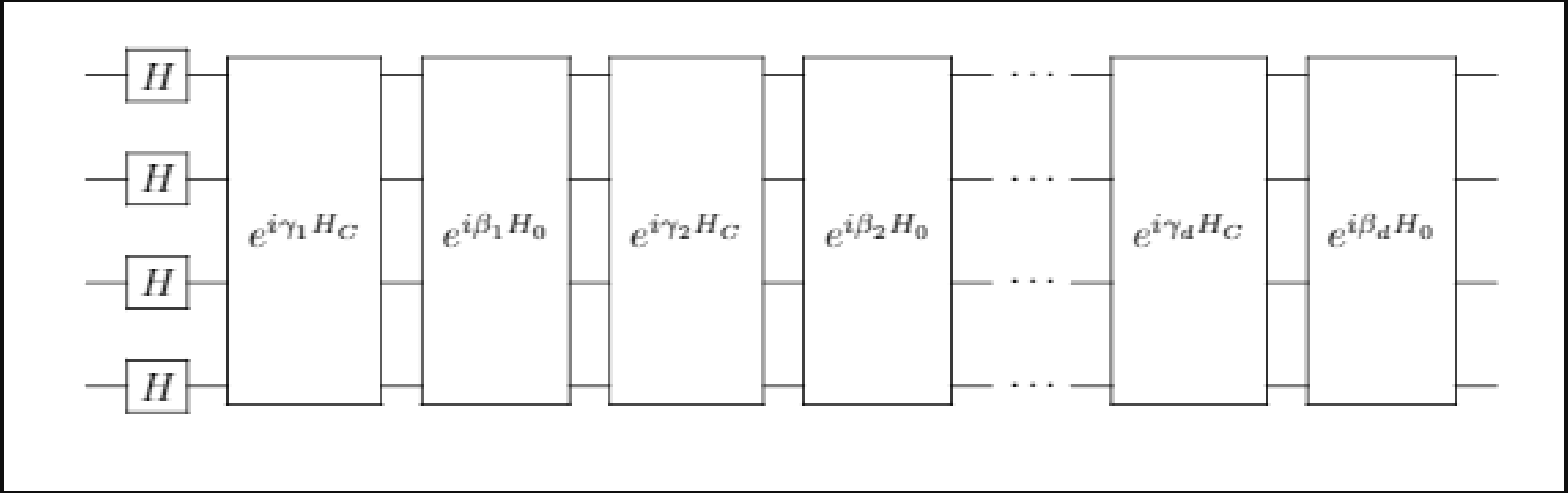
Solving combinatorial problems

- Introduced in 2014
- QUBO encoding



Quantum Approximate Optimization Algorithm

QAOA Circuit



Quantum Approximate Optimization Algorithm

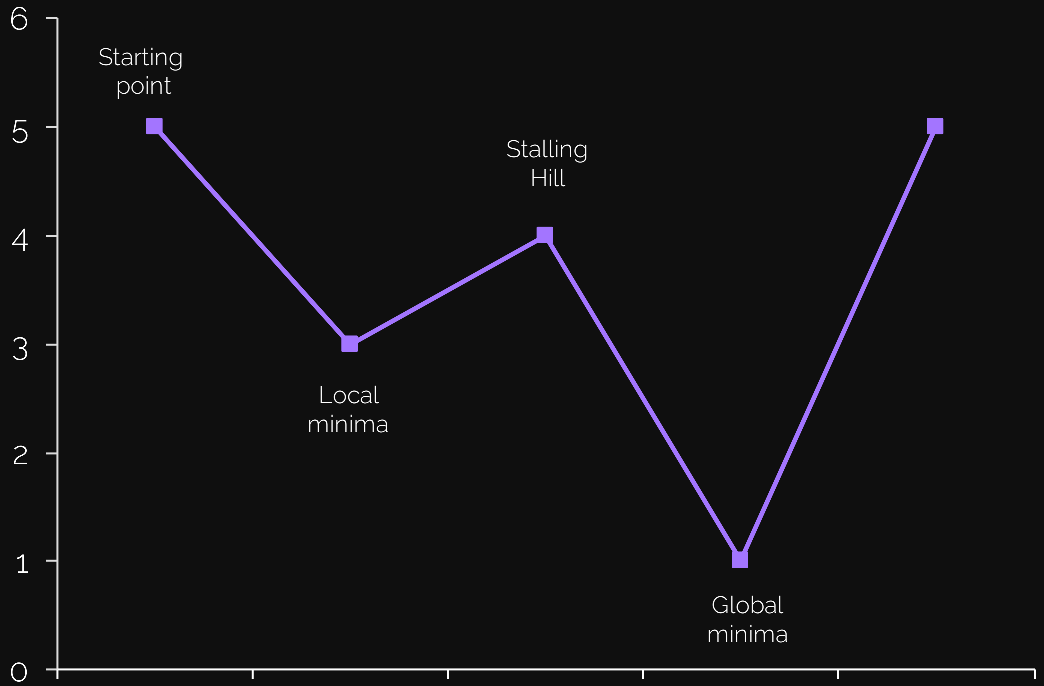
QAOA in practice

- Each vertex a qubit
- Each qubit in a partition
- Value of an edge based on his neighbours

Combinatorial problems

Solving combinatorial problems

- Simulated Annealing
- Simulated Quantum Annealing
- Quantum Annealing



03.

QAOA and Max-Cut, simulation through a QLM

Practical example on the use of our appliance

PyAQASM

A Python library to simplify

High level interface to design Quantum Circuits

Every bit of "tech" you need

Advanced usage for granular programming

Python

+

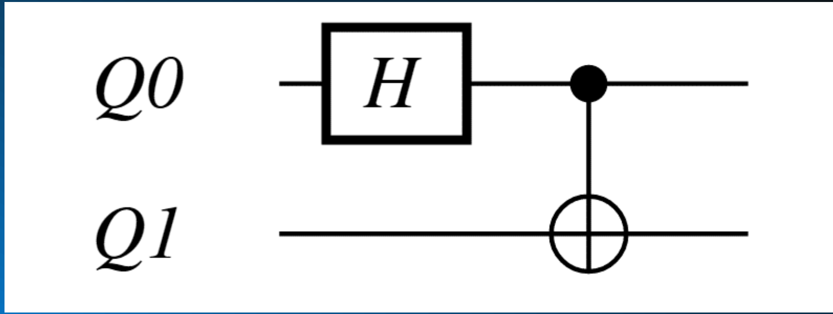
Atos QASM

Creating an EPR Pair

The circuit

- Represents a maximal entangled couple of qubits

- The output is always either $|00>$ or $|11>$



Creating an EPR Pair

The basics

- Program()
- .qalloc()
- .calloc()

```python
from qat.lang.AQASM import *
prog = Program()
```

Creating an EPR Pair

The basics

```
qub = prog.qalloc(2)
```

Creating an EPR Pair

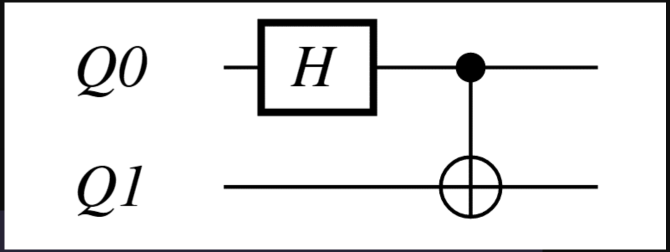
The basics

```
cb = prog.calloc(2)
```

Creating an EPR Pair

Populating the circuit

Gate calling




```
prog.apply(H, qub[0])

prog.apply(CNOT, qub[0], qub[1])
#CNOT(qub[0], qub[1])
```

Creating an EPR Pair

A peek to our circuit

- .to_circ()
- display / qat
- .to_job()
- .submit()

```
from qat.qpus import get_default_qpu
qpu = get_default_qpu()
result = qpu.submit(job)
```

Creating an EPR Pair

Showing the results

- Result
- Nbshots

```
result = qpu.submit(job)

for sample in result:
    print("State %s amplitude %s" % (sample.state, sample.amplitude))
```

Creating an EPR Pair

Showing the results

```python
job = circ.to_job(nbshots=10)
```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Circuits creation

The plugins

Alter the flow of our jobs, both in compiling and post process

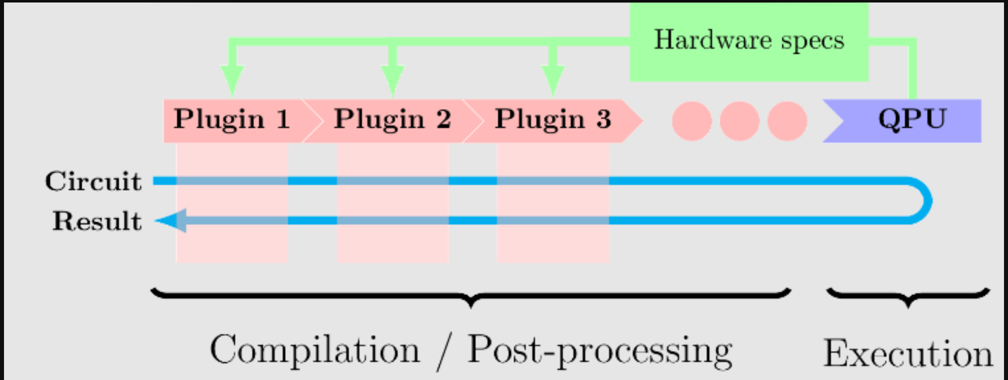
Simple and easy to use

You can even write your owns

Circuits creation
Building stacks

Put different plugins one after another

```
my_stack = plugin1 | plugin2 | .. | my_qpu
```



Circuits creation
The observables

- Used to determine the property of quantum states
- Automatize the sampling
- Can be manipulated

```
from qat.core import Observable, Term

obs1 = Observable(2, pauli_terms=[Term(1., "ZZ", [0, 1])])
obs2 = Observable(2, pauli_terms=[Term(1., "X", [0])])

print(obs1 + obs2)
```

Circuit creatrion

Parameterized circuits

- An hybrid Machine Learning circuit
- Unfixed gates
- Evolve the gates through computation

```
theta = prog.new_var(float, "\\theta")
prog.apply(RY(theta), qubits_reg[0])
```

QAOA on myQLM
The big picture

- CombinatorialProblem Class
- From problem to variational Ansätze
- Observable synthesis
- Circuit synthesis

QAOA on myQLM

CombinatorialProblem Class

- Problem and Variables
- Clauses
- Min and Max

```python
my_problem = CombinatorialProblem()

v0 = my_problem.new_var()
v_array = my_problem.new_vars(4)
```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QAOA on myQLM

CombinatorialProblem Class

- Problem and Variables
- Clauses
- Min and Max

```
print(v0 | v1)
print(~(v0 ^v_array[3] | v1))

my_problem.add_clause(v0 | v1, weight=2.)
```

QAOA on myQLM

CombinatorialProblem Class

- Problem and Variables
- Clauses
- Min and Max

```
my_maximization_problem = CombinatorialProblem(maximization=True)
```

QAOA on myQLM

CombinatorialProblem Class

```python
from qat.opt import CombinatorialProblem

my_problem = CombinatorialProblem()

v0 = my_problem.new_var()
v1 = my_problem.new_var()

v_array = my_problem.new_vars(4)

print(v0 | v1)
print(v_array[0] & v_array[2])
print(v0 ^ v_array[0])
print(~v0)
print(~(v0 ^v_array[3] | v1))

my_problem.add_clause(v0 ^ v1)

my_problem.add_clause(v0 | v1, weight=2.)
for clause, weight in my_problem.clauses:
    print(clause, weight)
```

```
V(0) V(1)
V(2), V(3), V(4), V(5)
V(0) | V(1)
V(2) & V(4)
V(0) ^ V(2)
~ V(0)
~ ((V(0) ^ V(5)) | V(1))
V(0) ^ V(1) 1.0
V(0) | V(1) 2.0
```

QAOA on myQLM

From problem to variational Ansätze

- Ansätze construction

```
depth = 3
ansatz = my_problem.qaoa_ansatz(depth).circuit
ansatz.display()

ansatz_gamma_0_pi = ansatz.bind_variables({"\\gamma_{0}": np.pi})
```

QAOA on myQLM

From problem to variational Ansätze

```python
depth = 3
ansatz = my_problem.qaoa_ansatz(depth).circuit
ansatz.display()

print("Variables:", ansatz.get_variables())

import numpy as np
ansatz_gamma_0_pi = ansatz.bind_variables({"\\gamma_{0}": np.pi})
```

QAOA on myQLM

Observable synthesis

- Encoding in smaller Hamiltonians

$$exp := exp \vee exp | exp \wedge exp | exp \oplus exp | \neg exp | V$$

$$H(e_1 \vee e_2) = H(e_1) + H(e_2) - H(e_1)H(e_2)$$

$$H(e_1 \wedge e_2) = H(e_1) * H(e_2)$$

$$H(e1 \oplus e2) = H(e1) + H(e2) - 2H(e1)H(e2)$$

$$H(\neg e) = 1 - H(e)$$

$$H(V(i)) = \frac{1-\sigma_i^z}{2}$$

QAOA on myQLM

Observable synthesis

- Encoding in smaller Hamiltonians

```
for i in range(4):
    my_problem.add_clause(variables[i]^variables[i+1])
print("Minimization:\n", my_problem.get_observable())
```

```
Minimization:
 2.0 * I^5 +
-0.5 * (ZZ|[0, 1]) +
-0.5 * (ZZ|[1, 2]) +
-0.5 * (ZZ|[2, 3]) +
-0.5 * (ZZ|[3, 4])
```

QAOA on myQLM
Observable synthesis

- Encoding in smaller Hamiltonians

```python
my_problem = CombinatorialProblem(maximization=True)
variables = my_problem.new_vars(5)
for i in range(4):
    my_problem.add_clause(variables[i]^variables[i+1])
print("Maximization:\n",my_problem.get_observable())
```

```
Maximization:
 -2.0 * I^5 +
0.5 * (ZZ|[0, 1]) +
0.5 * (ZZ|[1, 2]) +
0.5 * (ZZ|[2, 3]) +
0.5 * (ZZ|[3, 4])
```

QAOA on myQLM

Circuit synthesis

- Circuit synthesis algorithms

```
circuit1 = my_problem.qaoa_ansatz(1, strategy="default").circuit
circuit2 = my_problem.qaoa_ansatz(1, strategy="coloring").circuit
circuit3 = my_problem.qaoa_ansatz(1, strategy="gray_synth").circuit
```

QAOA on myQLM

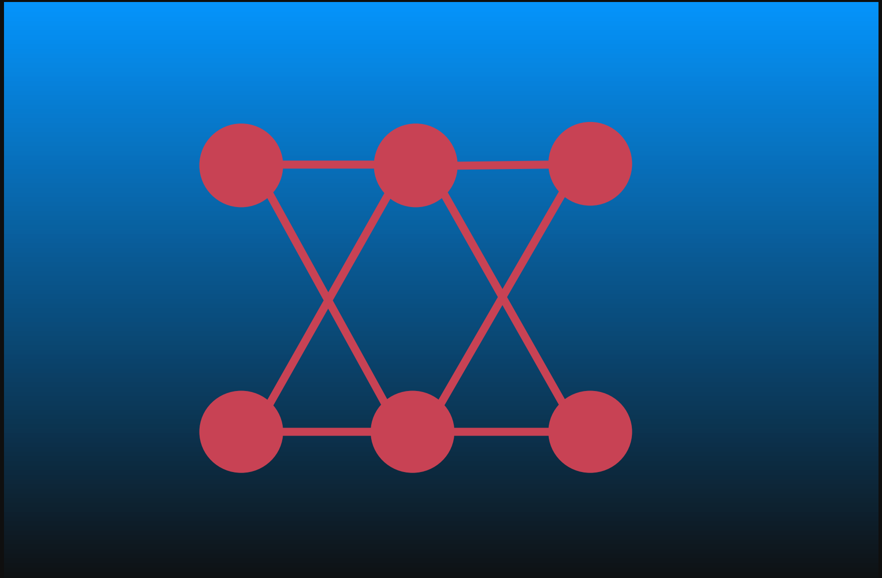
What exactly is a max-cut?

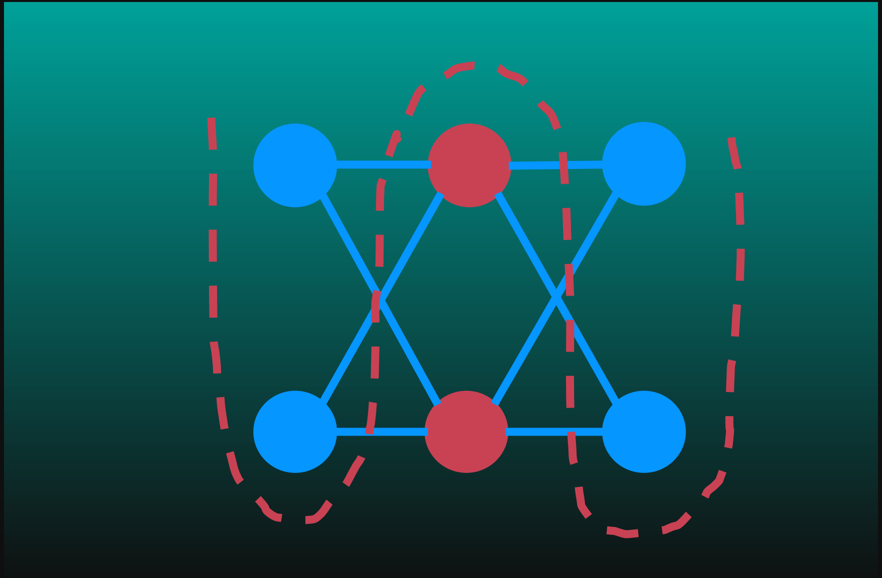
A graph partitioning problem:

- Cut our graph (G) in 2 subsets (S and V)
- Each subset must have a number > 0 of vertexes
- Maximize the number of edges crossed by the cut

QAOA on myQLM

What exactly is a max-cut?





QAOA on myQLM

Running of a MaxCut

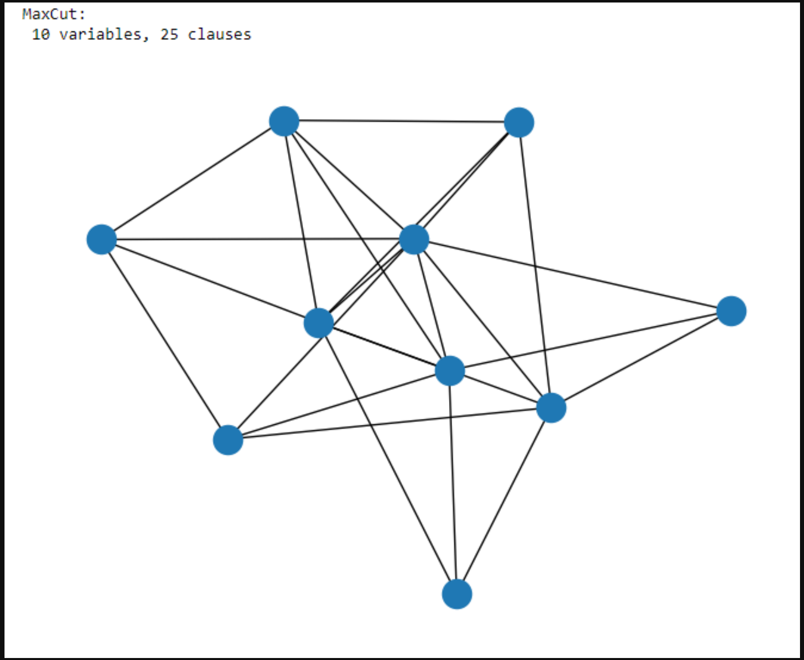
- Integrated wrapper
- Variational plugin to OPT

```python
import networkx as nx

graph = nx.generators.random_graphs.erdos_renyi_graph(10, 0.5)
nx.draw(graph)
from qat.vsolve.qaoa import MaxCut
problem = MaxCut(graph)
print(problem)
```

QAOA on myQLM

Running of a MaxCut

- Integrated wrapper
- Variational plugin to OPT



QAOA on myQLM

Running of a MaxCut

- Integrated wrapper
- Variational plugin to OPT

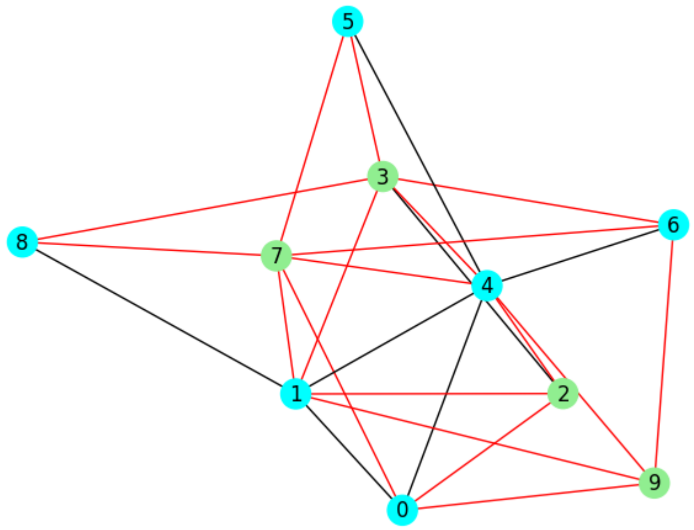
```python
from qat.qpus import get_default_qpu
from qat.plugins import ScipyMinimizePlugin
qpu = get_default_qpu()
stack = ScipyMinimizePlugin(method="COBYLA",
                            tol=1e-5,
                            options={"maxiter": 200}) | qpu

job = problem.qaoa_ansatz(3)
result = stack.submit(job)
print("Final energy:", result.value)
```

QAOA on myQLM

Running of a MaxCut

- Integrated wrapper
- Variational plugin to OPT

```
Most probable states are:
And as bitstrings:
Most probable cut: {0, 1, 4, 5, 6, 8} {9, 2, 3, 7}
```



myQLM

Click on the picture or visit
myqlm.github.io/notebooks

Thank you!

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