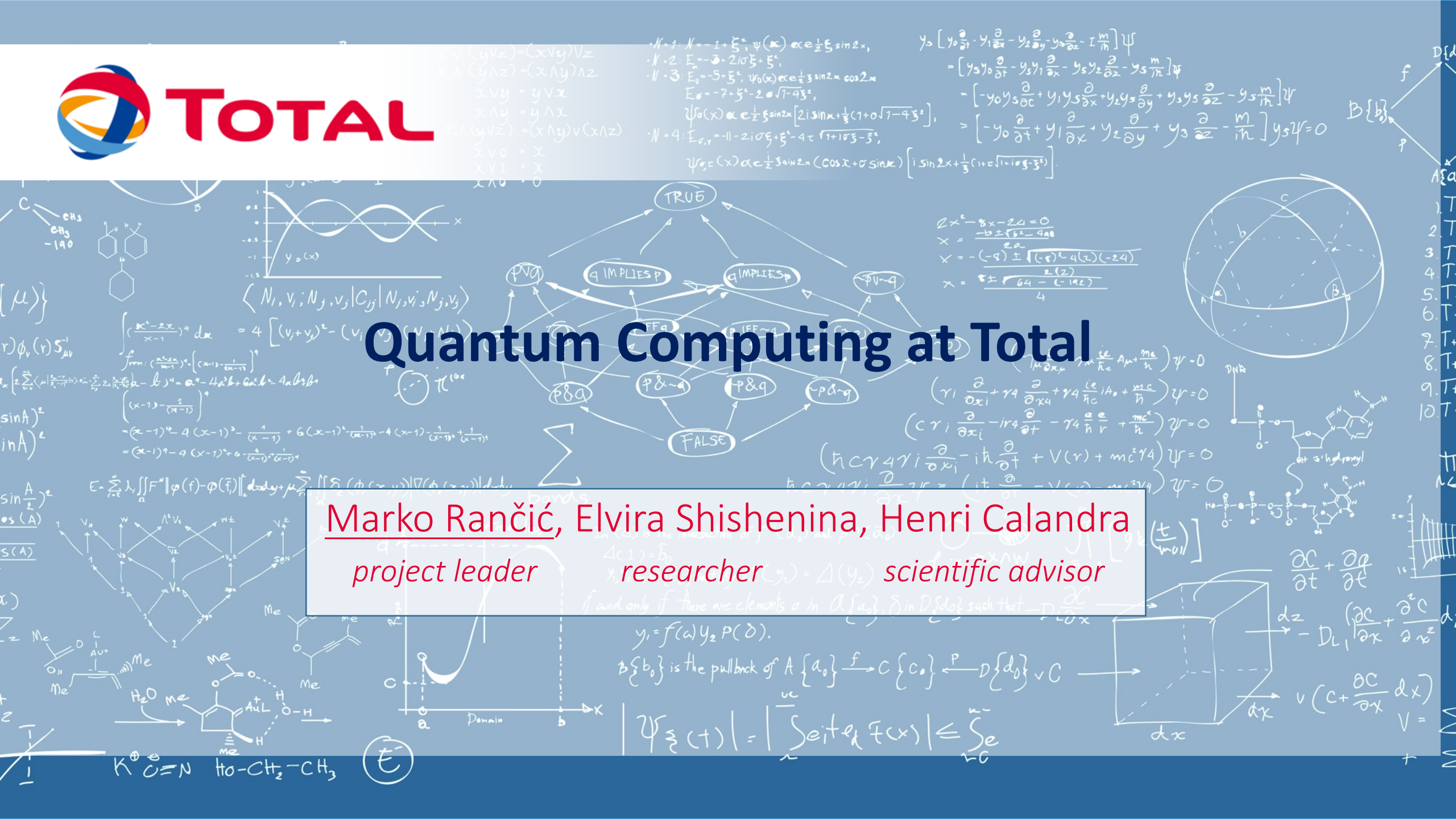
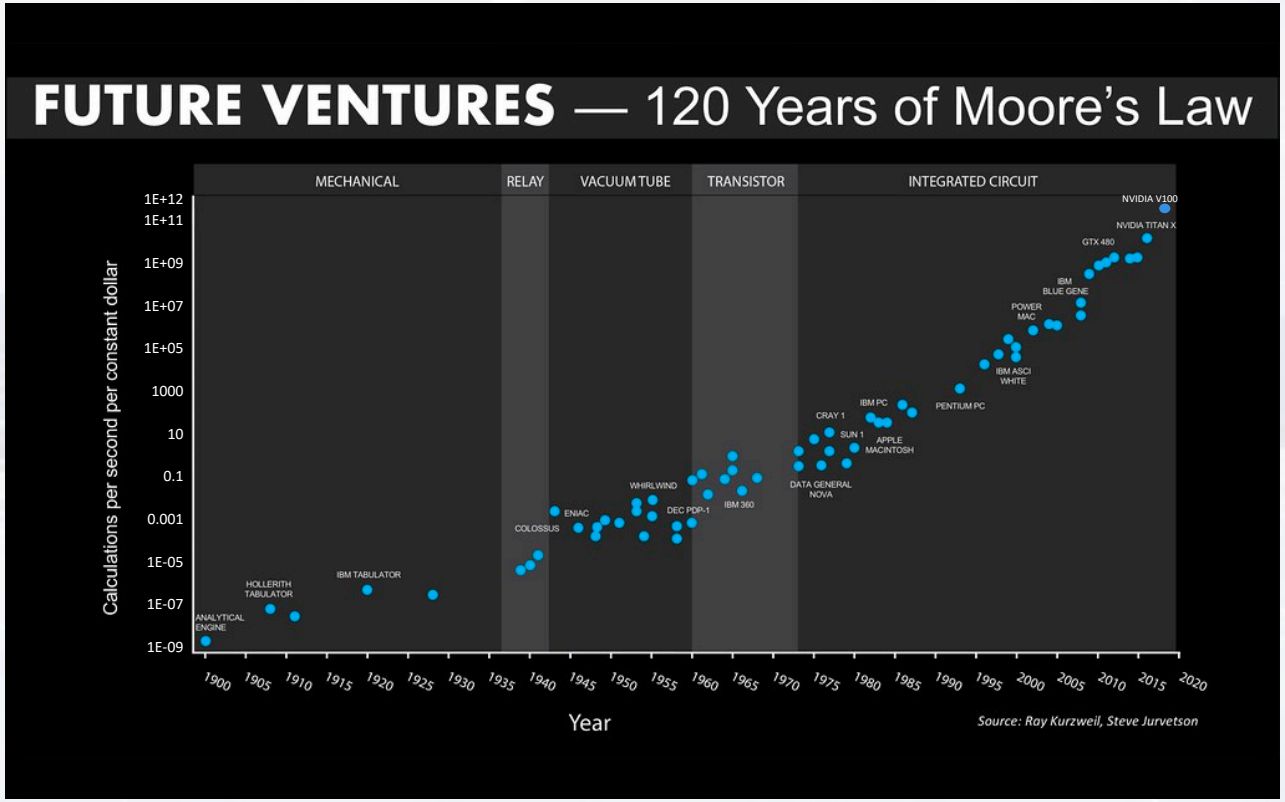


Quantum Computing at Total

Marko Rančić, Elvira Shishenina, Henri Calandra

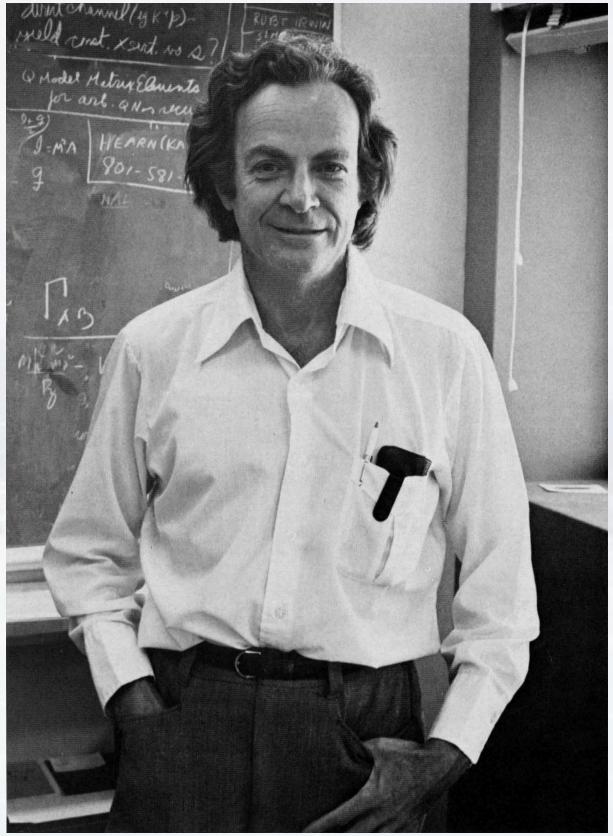
project leader *researcher* *scientific advisor*

Motivations



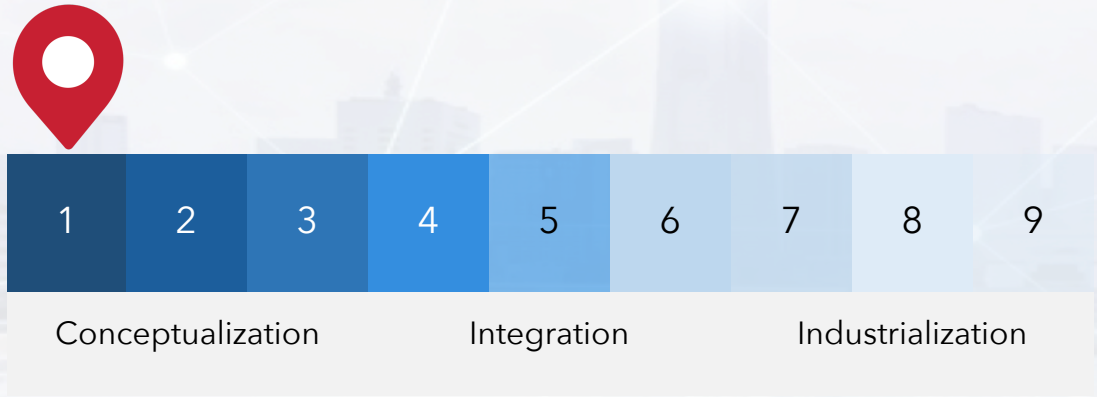
- Number of transistors in an IC doubles every 2 years
- end of Moore's law by around 2025

Motivations



Dashboard

we are here



Total's Role Leader/Catalyst

2019

- project leader and junior researcher recruitment
- 3 PostDocs + 3 PhD students
- from 30 qubits QLM up to 35 qubits QLM
- develop in-house experiences in QC algorithms
- Expand the industry and academy network
- Participate in EU proposals
- 2 papers
- Reach an agreement with a quantum hardware manufacturer

Industrial and academic network

ATOS 35 qubit Quantum Learning Machine

ATOS QLM scope

Programming

- **AQASM** — Assembly language to build quantum circuits
- **pyAQASM** — Python extension to AQASM
- **CIRC** — Binary format of quantum circuits
- **QLIB** — AQASM & pyAQASM libraries
- **INTEROP** — Connections with other frameworks

QPU

- **QPU** — Quantum processing unit emulation

Optimization

- **PBO** — Pattern based optimizer
- **Circuit Optimizer** — Generic circuit optimizer
- **NNIZER** — Topology constraint solver

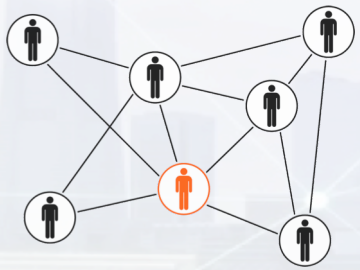
Simulation

- **SIMULATORS** — Simulation modules
- **SIM OPTIMIZER** — Best Simulator dynamic selection
- **PHYSICS** — Physical Noise models

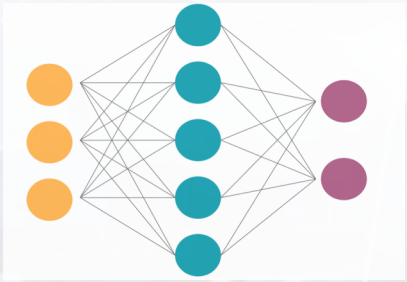
Bull Atos technologies (2018)

Roadmap & potentital use cases

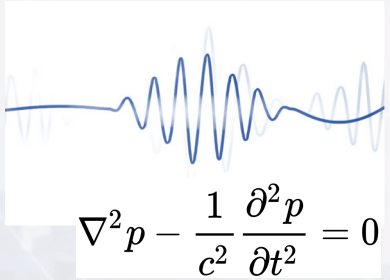
Quantum chemistry



Quantum combinatorial optimization



QML

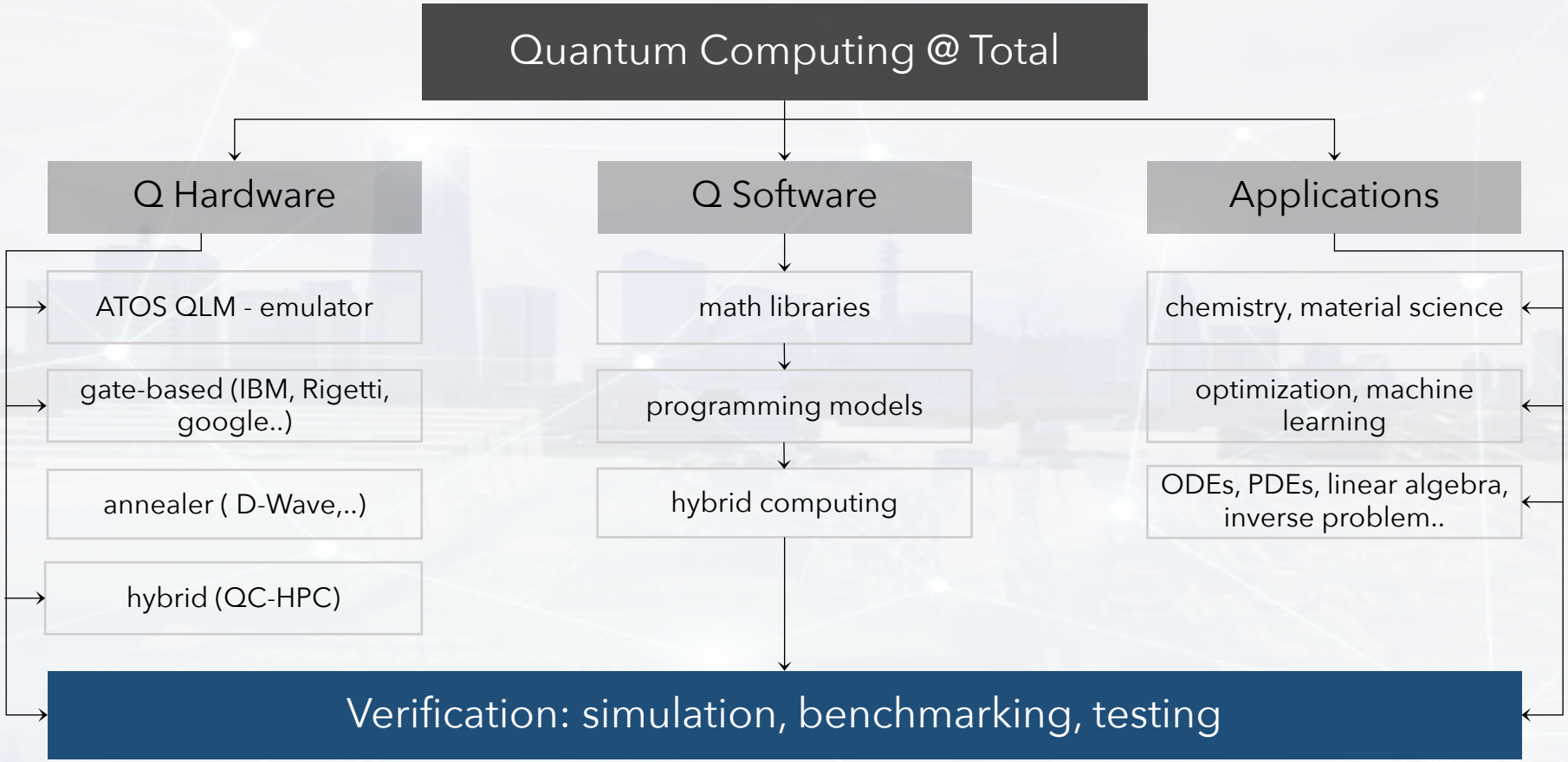


Linear algebra (ODEs, PDEs, inverse problems)

NISQ device ~ (10^2 qubits) 3-5 years

(pre)-QEC device ~ ($10^{3(-6)}$ qubits) 5++ years

Global program overview



Quantum Chemistry ground state problem with VQE

A.Peruzzo et al. A variational eigenvalue solver on a quantum processor (2014). arXiv:1304.3061

Ritz variational method

$$H|\Psi_{\text{exact}}(\beta_1; \ldots \beta_n)\rangle = E_{\text{exact}}|\Psi_{\text{exact}}(\beta_1; \ldots \beta_n)\rangle$$

Ritz variational method

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$$|\Psi_{\text{guess}}(\alpha_1; \ldots \alpha_n)\rangle$$

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$$|\Psi_{\text{guess}}(\alpha_1;\ldots\alpha_n)\rangle$$

$$E_{\text{g.s.}} \leq \frac{\langle\Psi_{\text{guess}}(\beta_1;\ldots\beta_n)|H|\Psi_{\text{guess}}(\beta_1;\ldots\beta_n)\rangle}{\langle\Psi_{\text{guess}}(\beta_1;\ldots\beta_n)|\Psi_{\text{guess}}(\beta_1;\ldots\beta_n)\rangle}$$

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?????

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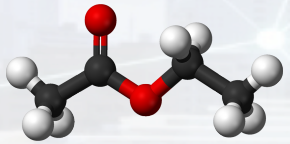
TOTAL

VQE | design

fermionic problem



?????

qubit Hamiltonian

$$H_q = \sum_\alpha h_\alpha P_\alpha$$

Oh now I understand the question

optimize

prepare trial state QPU

$$|\Psi(\boldsymbol{\theta})\rangle$$

measure expectation value

$$h_\alpha \langle \Psi(\boldsymbol{\theta}) | P_\alpha | \Psi(\boldsymbol{\theta}) \rangle$$

calculate energy CPU

$$E_q(\boldsymbol{\theta}) = \langle \Psi(\boldsymbol{\theta}) | H_q | \Psi(\boldsymbol{\theta}) \rangle = \sum_\alpha h_\alpha \langle \Psi(\boldsymbol{\theta}) | P_\alpha | \Psi(\boldsymbol{\theta}) \rangle$$

adjust parameters

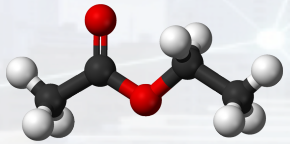
$$(\boldsymbol{\theta})$$

solution

$$E_q^{\min}$$

VQE | design

fermionic problem



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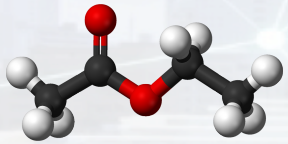
VQE | design

fermionic problem



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VQE | design

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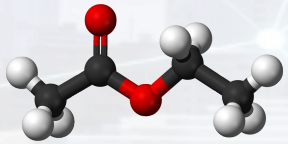

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adjust parameters

$$(\boldsymbol{\theta})$$

solution

$$E_q^{\min}$$

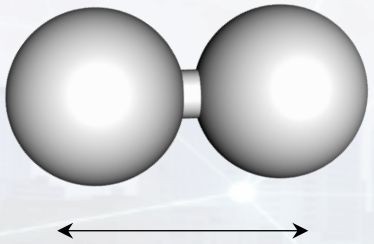
VQE | design

VQE library

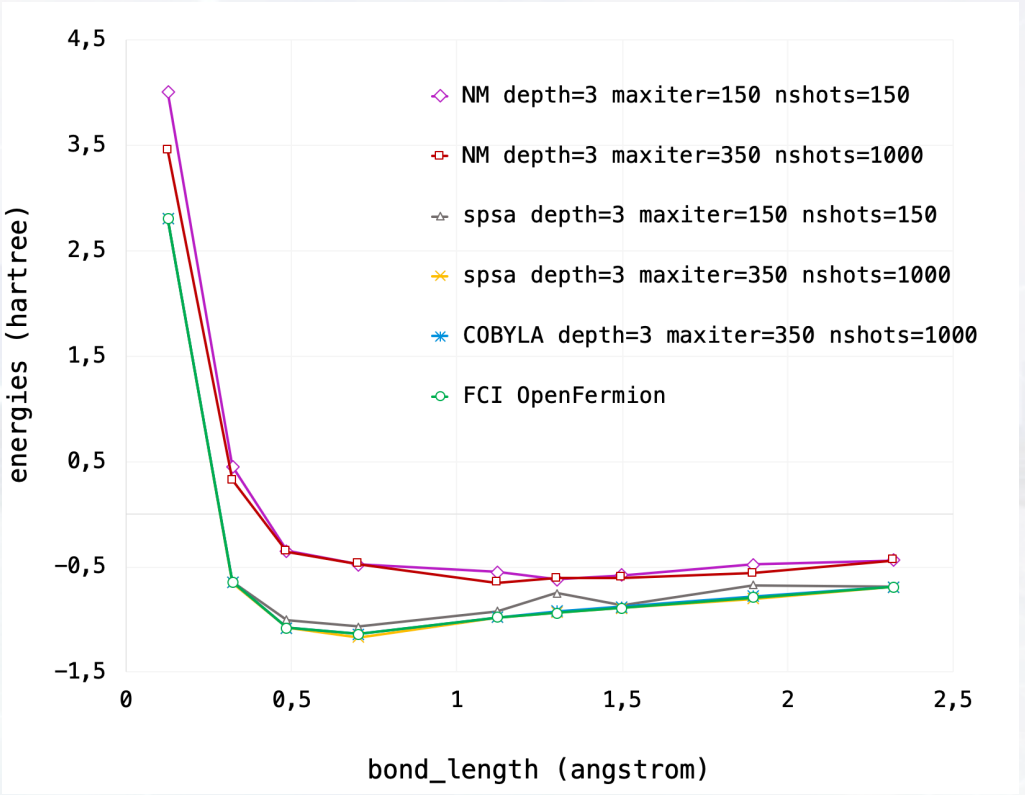
```python
from qat.linalg import get_qpu_server
from molecular_vqe.vqe import VQE
from molecular_vqe.ansatz import RYRZ
qpu = get_qpu_server

# define VQE parameters
number_qubit = 10
depth = 3
num_shots = 500
maxiter = 500
minimizer = 'COBYLA'

ansatz_ryrz = RYRZ(number_qubit, depth=depth)
vqe = VQE(number_qubit, qpu, openfermion_dict,
          ansatz_ryrz, minimizer=minimizer,
          num_shots=num_shots, maxiter=maxiter)

# run VQE
param_run = np.random.rand(ansatz_ryrz.get_num_parameters())
energy = vqe.run_minimize(init_params = param_run)


```

VQE | benchmarking

H2

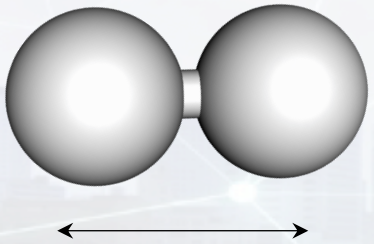


```
bond_length

charge = 0
multiplicity = 1
basis = 'sto-3g'
number_qubit = 4  # bravyi-kitaev
```



VQE | benchmarking

H2



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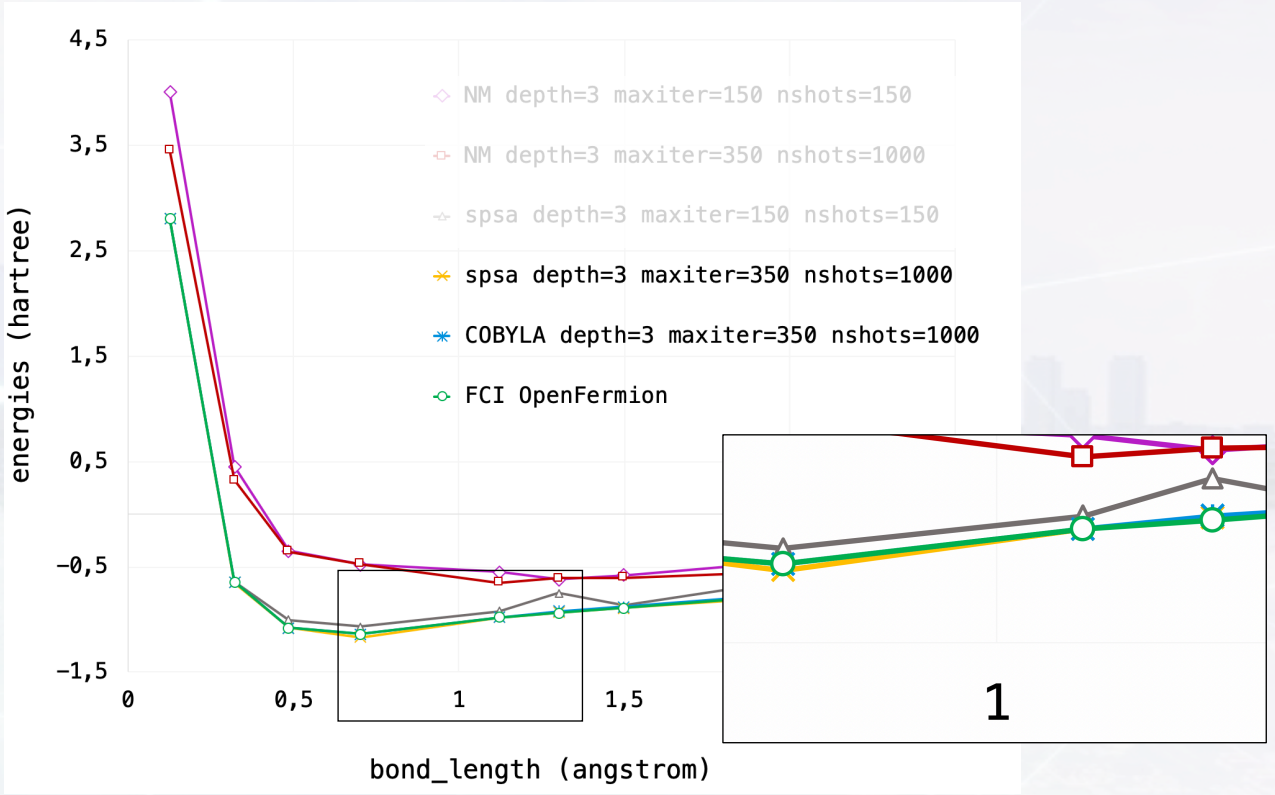
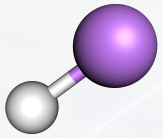
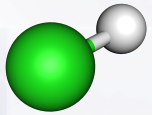
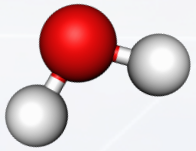
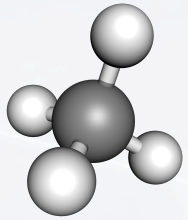
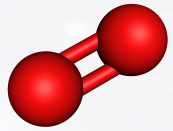
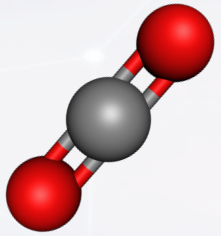
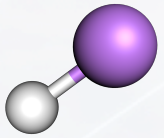
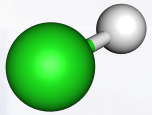
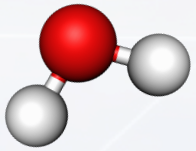
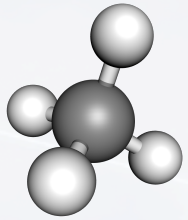
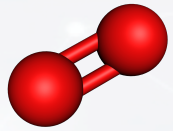
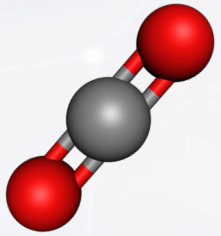


VQE | benchmarking

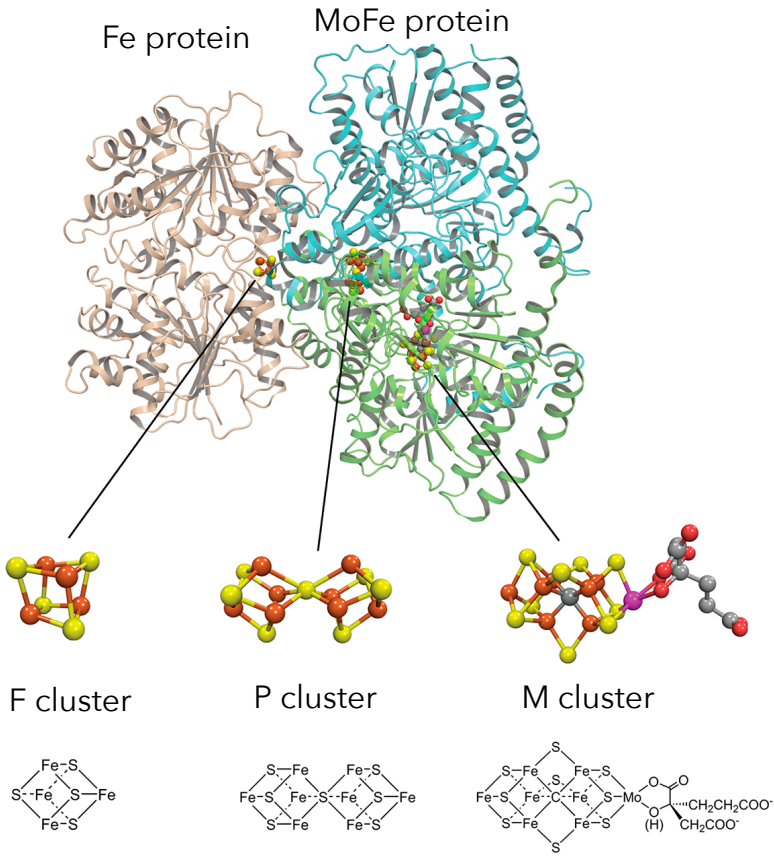
configuration						
	LiH	BeH	H2O	CH4	O2	CO2
num_orbitals	6	6	7	9	10	15
num_qubit	12	12	14	18	20	24*
num_shots	500	500	500	500	500	500
maxiter	350	350	350	350	350	350

VQE | benchmarking

ground state energies						
	LiH	BeH	H2O	CH4	O2	CO2
VQE Total	-7.76	-14.44	-72.91	-38.97	-144.28	-179.93
VQE Atos	-7.79	-14.60	-73.15	-39.12	-144.15	-180.92
FCI OpenFermion	-7.87	-14.96	-74.99	-39.81	-147.74	-185.23

1 - 3 % difference with respect to classical algorithms

VQE | benchmarking



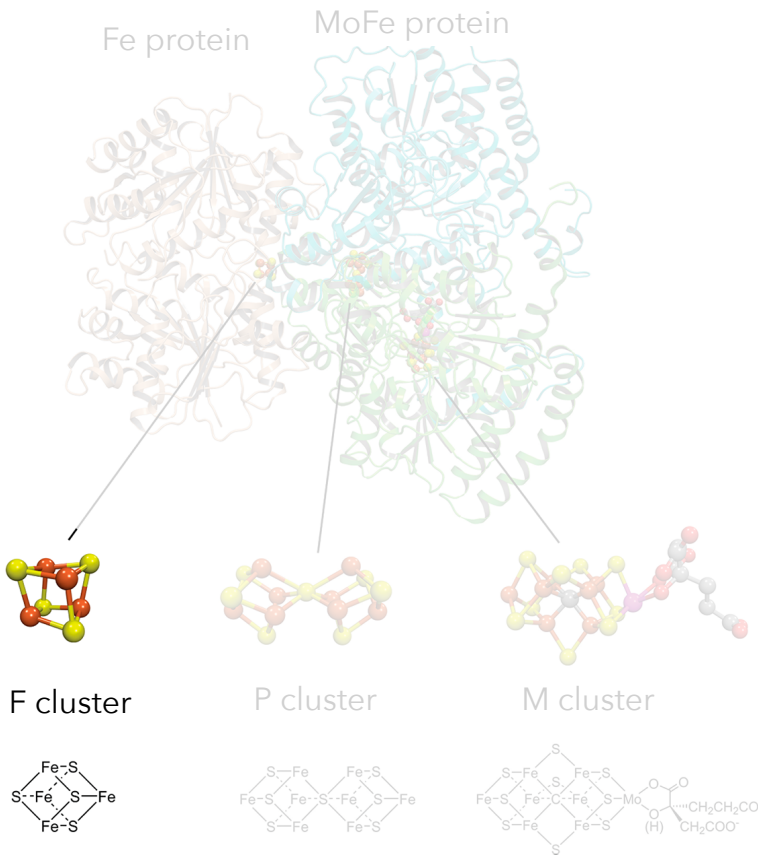
Molybdenum nitrogenase

—— Iron sulfide clusters (Fe_S_) of different sizes

B.Hoffman et al. Mechanism of nitrogen fixation by nitrogenase (2014). dx.doi.org/10.1021/cr400641x

VQE | benchmarking

Simulating F cluster is at the limit of classical computers! *(IBM Research, 2018)*



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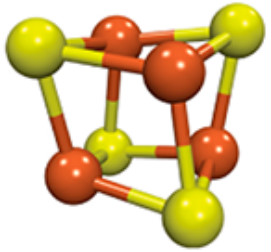
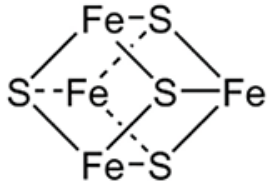
TOTAL

VQE | benchmarking



F cluster



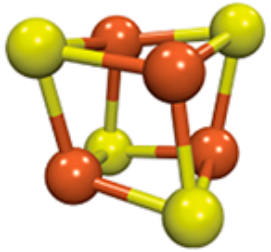
4Fe - 4S

4 x 26 + 4 x 16 = 168 electrons

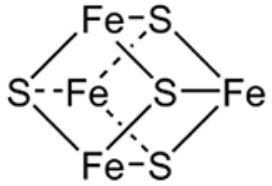
~ 10^50 permutations

TOTAL

VQE | benchmarking



F cluster



4Fe - 4S

4 x 26 + 4 x 16 = 168 electrons

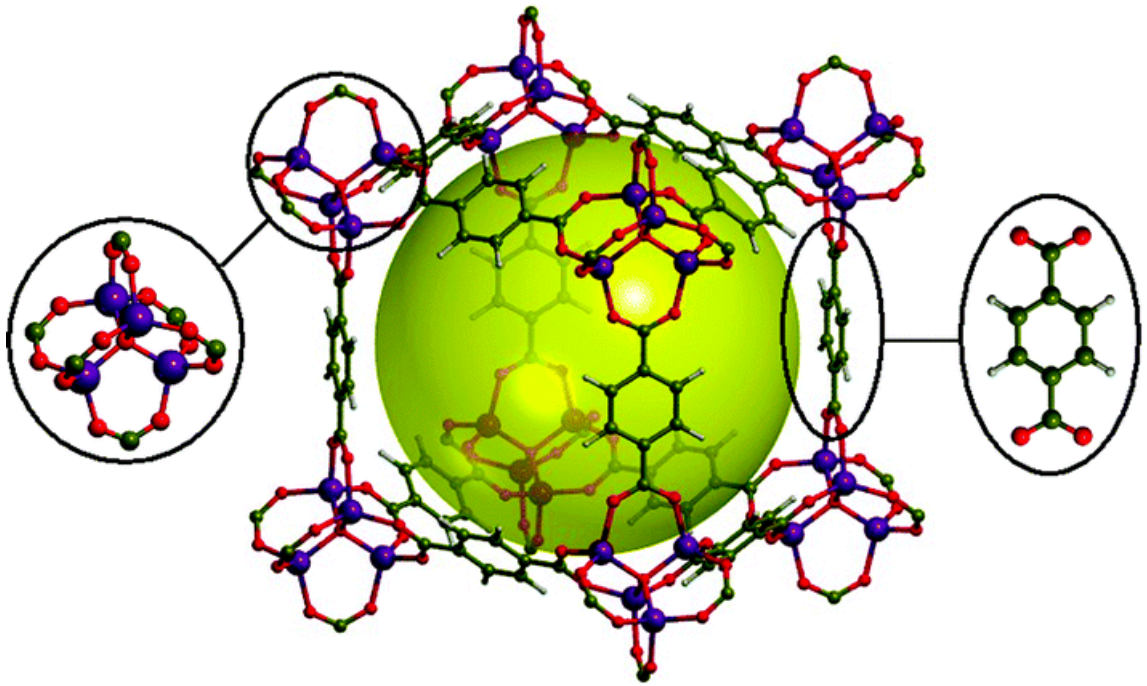
~ 10^50 permutations

~ 192 qubits

(3-5 years)

TOTAL

VQE | holy grail



CrystEngComm,8, 364-371 (2006(

Quantum Combinatorial Optimization

with V. Dunjko and C. Moussa from Leiden

- **Knappsack problem** (Function Maximization with Dynamic Quantum Search. In International Workshop on Quantum Technology and Optimization Problems (pp. 86-95). Springer, Cham.

- **MaxCut and QAOA (manuscript in preparation)**

- Scheduling, Traveling Salesman

TOTAL

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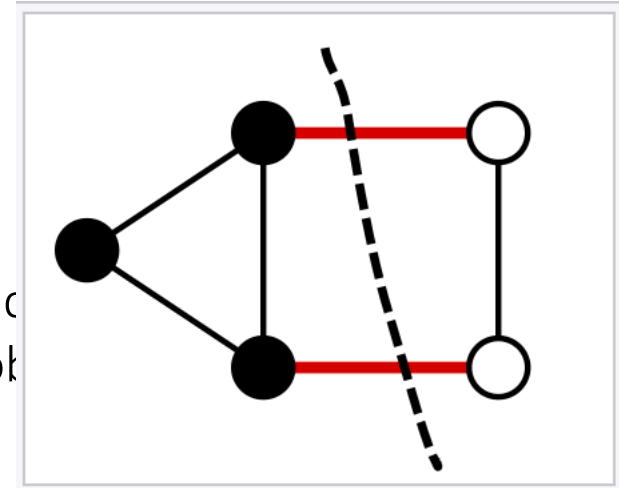
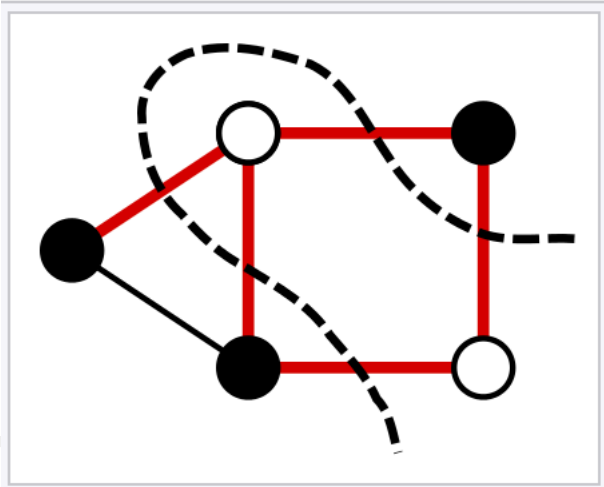


A minimum cut.



A maximum cut.

TOTAL

QAOA

A graph MaxCut algorithm

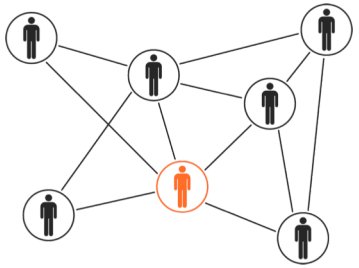
$$G = (V, E)$$

Map a matrix of a graph to an Ising like Hamiltonian

$$H_{\mathrm{C}} = \sum_{\langle ij \rangle \in E} \frac{w_{ij}}{2} \sigma_i^z \sigma_j^z \qquad H_{\mathrm{B}} = \sum_{j=1}^{n} \sigma_j^x$$

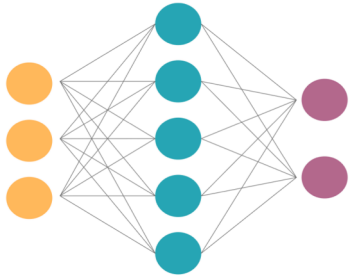
$$|\gamma, \beta\rangle = e^{-i\beta_p H_{\mathrm{B}}} e^{-i\gamma_p H_{\mathrm{C}}} \ldots e^{-i\beta_1 H_{\mathrm{B}}} e^{-i\gamma_1 H_{\mathrm{C}}} |+\rangle^{\otimes n}$$

$$F_p(\gamma, \beta) = \langle \gamma, \beta | H_{\mathrm{C}} | \gamma, \beta \rangle$$

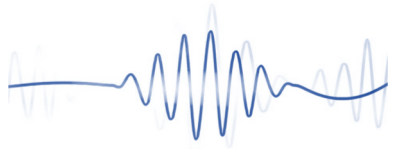


TOTAL

ML and PDE's



Hydrocarbon well modelling



$$\nabla^2 p - \frac{1}{c^2}\frac{\partial^2 p}{\partial t^2} = 0$$

Seismic depth imaging (sesmic wave Eq.)

Quantum computing in 2020 at TOTAL

- Investigating the scalability of VQE + investigate further algorithms for chemistry
- Continue investigating combinatorial optimization (traveling salesman)
- Find more exciting avenues to explore with quantum computing: differential equations, machine learning (pattern recognition)
- Run alhorithms on actuall hardware

Quantum computing in the next 5 years

- TOTAL is the global leader in quantum algorithm design

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