

# Near-term QC applications in industry

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Material Simulation >

< Battery Optimization

# REQUIRED DEFINITION: USEFUL QUANTUM SUPREMACY

Quantum supremacy: proof that quantum computing can perform a particular calculation that's beyond the reach of any conventional computer. For the universal quantum computer and **certain problems**, this is supposed to be achieved with ~50 logical qubits. Universal quantum computers will also allow for the simulation of quantum particles, which is required for solving particular materials optimization problems involving large-scale quantum behavior.

We prefer to talk about **useful quantum supremacy**, because only when we solve real-world problems, it makes sense for VW.

# QUANTUM-ASSISTED ALGORITHMS

Currently, certain hardware constraints are given:

- Up to 50 physical qubits for universal quantum computers by the end of 2017/ early 2018
- ~2.000 qubits on quantum annealing systems

Most promising right now:

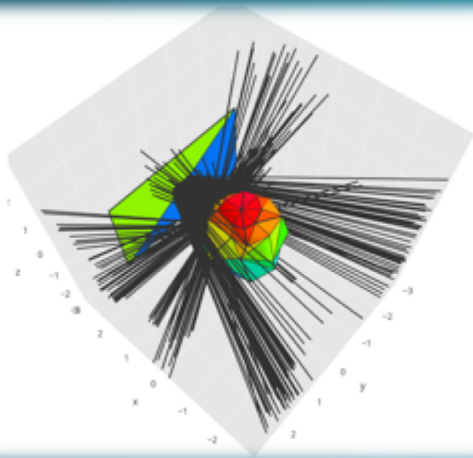
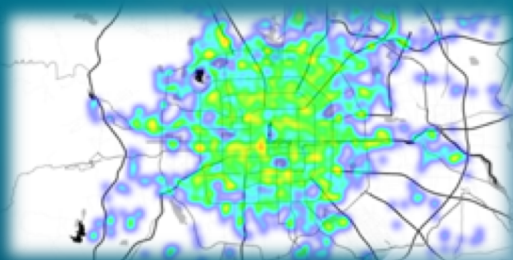
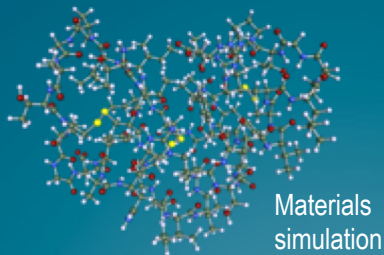
- Quantum-assisted machine learning
- Augmentation of deep learning, reinforcement learning, optimization algorithms and sampling
- Quantum simulation

		Type of algorithm	
		classical	quantum
Type of data	classical	CC	CQ
	quantum	QC	QQ

- First letter: system under study is classical or quantum
- Second letter: classical or quantum information processing device is used

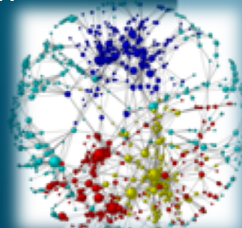
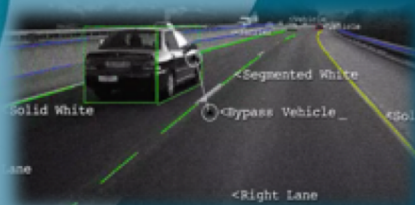
# WHAT'S HAPPENING AT VW (1)

With classical computers, many of the most complex problems can't be solved.



Quantum annealing – some things we've done so far

- Traffic flow optimization
- Reinforcement learning (i.e. financial market prediction, self-driving vehicle)
- Finite elements
- Machine learning (i.e. neural networks, NMF)
- Clustering (i.e. IT threat detection)
- Vehicle price prediction
- Vehicle weight minimization



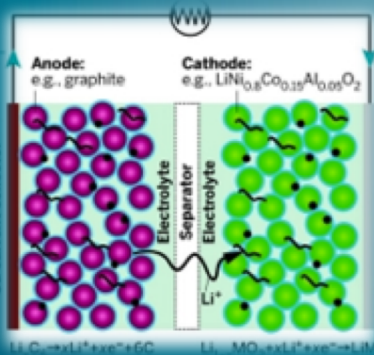
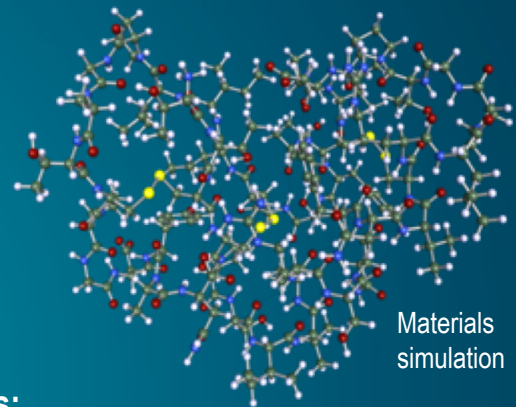




# WHAT'S HAPPENING AT VW (2)

## Gate model – we are working on

- Optimization (i.e. enhancing traffic flow optimization)
- Machine learning (i.e. quantum neural networks, financial market analysis)
- Simulation for possible discovery of new materials (i.e. battery materials)



## Additional results:

- 5 academic R&D partnerships, mostly pro bono
- Commercial partnerships with Google, D-Wave
- Presentations received at 9 conferences
- Publications pending in leading scientific journals



# TRAFFIC FLOW OPTIMIZATION AND ACTUAL STATUS

Full publication and description at <https://www.frontiersin.org/articles/10.3389/fict.2017.00029/full>

## Why quantum?

- Recalculation happens almost instantaneously.
- What we achieve: maximization of flux at any time.

## Actual status and next steps

- Electrify America – optimization of routes under consideration of charging pillars.
- Include additional optimization targets, and ideally work together with cities.
- Reduction of accidents, prediction and avoidance of „danger zones“ (insurance?), reduction of emissions.





# QUANTUM-ASSISTED REINFORCEMENT LEARNING

Full publication and description at <https://www.frontiersin.org/articles/10.3389/fphy.2017.00071/full>

## Reinforcement learning and motivation

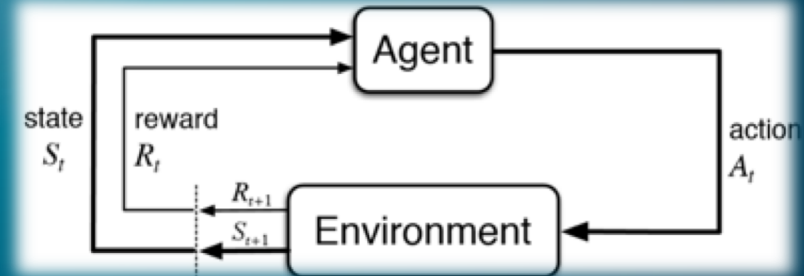
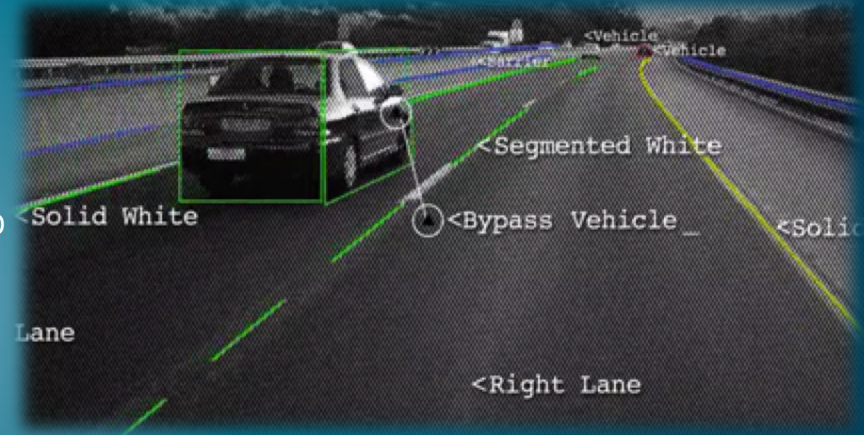
- Rewarding good results, i.e., simulating millions of parking maneuvers and rewarding successful ones.
- Agents, such as self-driving vehicles, intend to find the best thing to do in a given situation to reach their goal (parking, maneuvering through traffic, etc.) – they learn by trial and error.

## Goal: the closer to the real-world simulations are, the better the results

- As the world is dynamic, the agent may need to consider new observations/ data it hasn't seen before and adapt it's strategy.
- Given time-constraints, quantum-enhanced reinforcement learning has the potential to help agents analyze and learn quicker

## Next steps

- Apply to far more complex real-world scenarios





# QUANTUM-ASSISTED CLUSTERING

Full publication and description at <https://arxiv.org/abs/1803.02886>

## Motivation

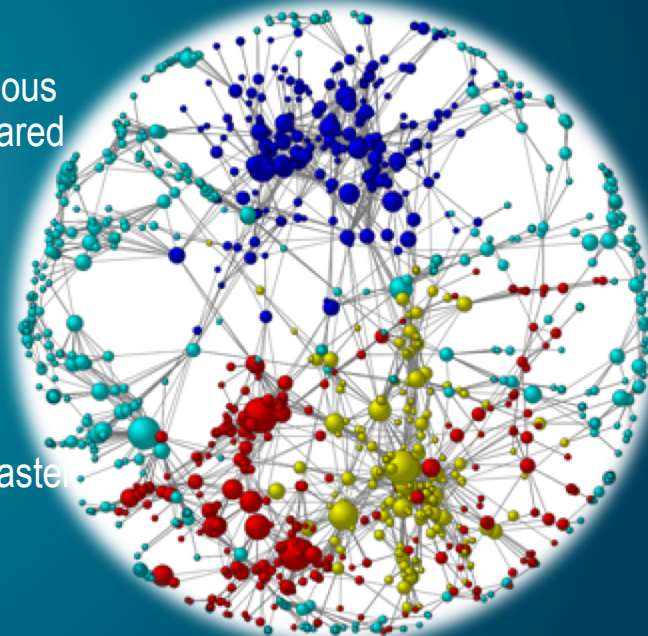
- Clustering is useful in a variety of applications, especially for uncovering and understanding network behavior, i.e.:
  - model how something can move through a network. For example, malicious software will propagate more quickly through a dense community, compared to a sparse one
  - extrapolate insight about organizational structures from complex communications meta-data
  - look at clusters of fraudulent activity

## Goal

- Invent a quantum-enhanced clustering algorithm that's more accurate and faster than purely classical clustering algorithms

## Actual status and next steps

- First, quantum-enhanced clustering algorithm in place
- Application to complex real-world scenarios, i.e., cyber security







# Quantum Artificial Neural Network (1)

## Motivation

- Artificial neural networks may be used whenever software cannot be explicitly programmed to solve a task (or only with significant effort).
- Optimize a performance criterion using example data or past experience.

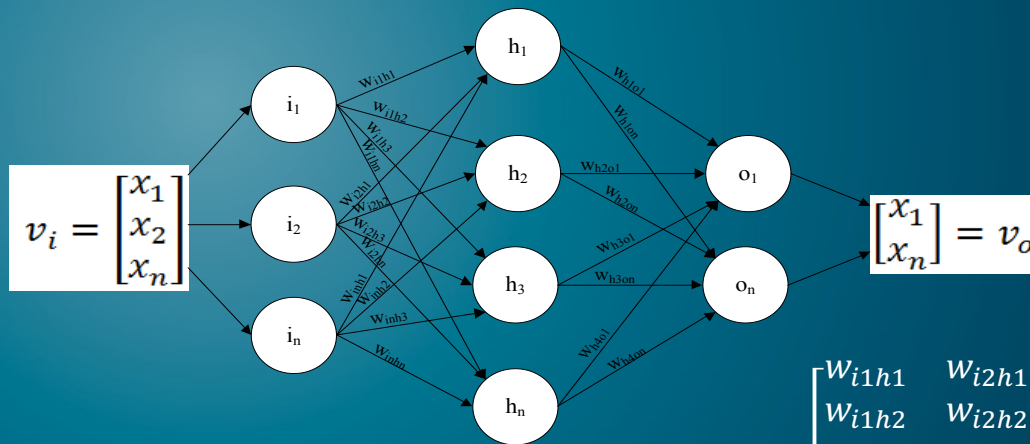
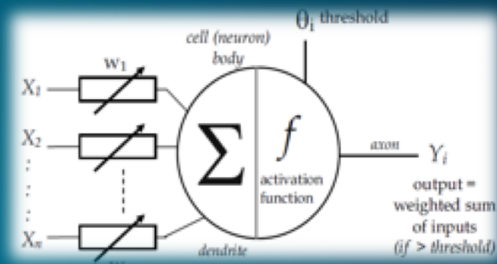
## Goal

- Implement a QNN and verify if either performance or accuracy can be improved compared to a classical ANN.

## Actual status

- First QNN in place.
- Application to complex real-world scenarios, i.e., MNIST data set.

$$m_{ho} = \begin{bmatrix} w_{h1o1} & w_{h2o1} & w_{h3o1} & w_{hno1} \\ w_{h1on} & w_{h2on} & w_{h3on} & w_{hnon} \\ t_1 & t_2 & t_3 & t_4 \end{bmatrix}$$



$$x_t = h_2 \left( w_0 + \sum_{j=1}^l w_j h_1 \left( w_{0j} + \sum_{i=1}^p w_{ij} x_{t-i} \right) \right) + \epsilon_t$$

$$m_{ih} = \begin{bmatrix} w_{i1h1} & w_{i2h1} & w_{inh1} \\ w_{i1h2} & w_{i2h2} & w_{inh2} \\ w_{i1h3} & w_{i2h3} & w_{inh3} \\ w_{i1hn} & w_{i2hn} & w_{inhn} \\ t_1 & t_2 & t_3 \end{bmatrix}$$



# Quantum Artificial Neural Network (2)

- The D-Wave solves

$$Obj(x, Q) = x^T \cdot Q \cdot x$$

where  $x$  is the input vector, and  $Q$  describes the relation between the variables.

- Existing quantum-assisted ANN approaches sample the weight space.
- In our approach, we represent samples, weights and target variables as matrix and evaluate different configurations of the QNN in one annealing cycle.

## Next steps

See what this approach can be used for:

- Weight initializer for classical ANN training
- Full ANN trainer
- Train on MNIST

A very, very simple example

$$Xw = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} 0 \\ w_1 \\ w_2 \\ w_1 w_2 \end{bmatrix} = \hat{y}$$

$$Xw = \hat{y}$$

$$X^T X w = X^T \hat{y}$$

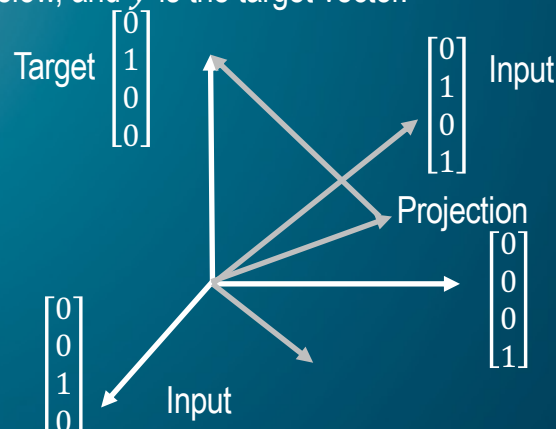
$$w = (X^T X)^{-1} X^T \hat{y}$$

$$Xw = X(X^T X)^{-1} X^T \hat{y} = Q \hat{y}$$

$$\arg \min_w Q \hat{y}$$

If  $\hat{y}$  is a free vector,  $Q \hat{y}$  is not free but its components are.  $Q$  is a projection operator as described below, and  $\hat{y}$  is the target vector.

We represent  $Q \hat{y}$  for different weight vectors on the chip at once. For a simple QNN, we tested it for up to 20 QNNs at once.





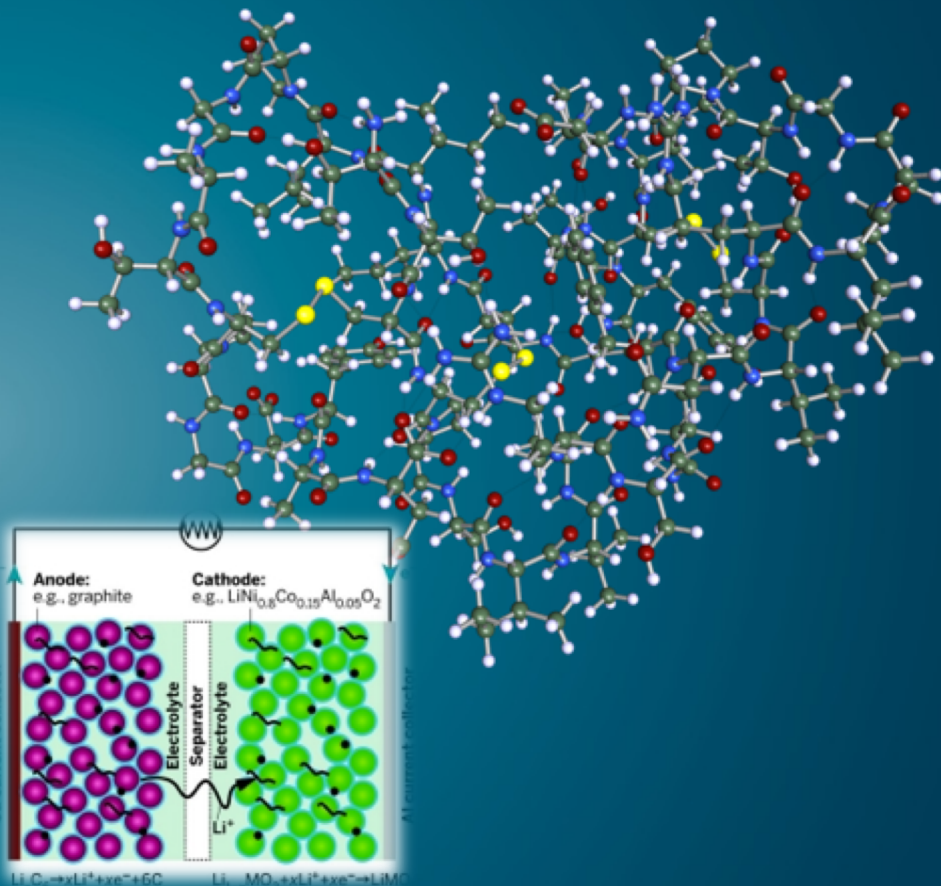
# ELECTRONIC STRUCTURE CALCULATIONS (1)

## Motivation

- With classical computers our calculations describe properties such as a molecule's ground-state energy by using the Schrödinger equation to calculate mathematical parameters called wave functions.
- Classical computers can solve such problems exactly only for elementary molecules because of the great complexity of the many interactions of the multiple subatomic particles found in larger compounds.
- Exact solutions rapidly become unfeasible, even for the fastest computers working over the entire lifetime of the universe.
- Quantum computers do not require exponentially increasing time to solve larger and larger systems, so they do not suffer the same limitations.

## Goal

- Find advanced materials





# ELECTRONIC STRUCTURE CALCULATIONS (2)

- Electronic structure problems are mainly targeted by gate model approaches
- Different quantum algorithms, as the variational quantum Eigensolver (VQE) or the phase estimation algorithm (PEA), were developed to find the ground state of small molecules
- But: current gate model devices suffer from different challenges:
  - Small number of qubits
  - Decoherence effects
  - Imperfect qubits and gates

- Molecules can be described by a fermionic Hamiltonian

$$H = \sum_{i,j} h_{ij}(R) a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} h_{ijkl}(R) a_i^\dagger a_j^\dagger a_k a_l$$

- $h_{ij}(R)$  and  $h_{ijkl}(R)$  are the one- and two-electron integrals for a specific interatomic distance  $R$ ,  $a_i^\dagger$  and  $a_i$  are the fermionic creation and annihilation operators
- As quantum devices use qubits, we have to map the fermionic operators onto qubit operators (e.g. by Jordan-Wigner transformation)

$$H = \sum_{i,\alpha} h_{\alpha}^i \sigma_{\alpha}^i + \sum_{i,j,\alpha,\beta} h_{\alpha\beta}^{ij} \sigma_{\alpha}^i \sigma_{\beta}^j + \sum_{i,j,k,\alpha,\beta,\gamma} h_{\alpha\beta\gamma}^{ijk} \sigma_{\alpha}^i \sigma_{\beta}^j \sigma_{\gamma}^k + \dots$$





# ELECTRONIC STRUCTURE CALCULATIONS (3)

- Hamiltonian consisting of qubit operators only, but how to map it on a QUBO?

- $\sigma_x, \sigma_y$  and  $\sigma_z$  terms instead of  $\sigma_z$  terms only
- $k$ -local terms instead of 2-local

- Below we show how to map such a  $n$ -qubit Hamiltonian with  $\sigma_x, \sigma_y$  and  $\sigma_z$  terms to a  $rn$ -qubit Hamiltonian with  $\sigma_z$  terms only

$$\sigma_x^i \rightarrow \frac{1 - \sigma_z^{i_j} \sigma_z^{i_k}}{2} S'(j) S'(k) \quad \sigma_y^i \rightarrow i \frac{\sigma_z^{i_k} - \sigma_z^{i_j}}{2} S'(j) S'(k)$$

$$\sigma_z^i \rightarrow \frac{\sigma_z^{i_j} - \sigma_z^{i_k}}{2} S'(j) S'(k) \quad I^i \rightarrow \frac{1 + \sigma_z^{i_j} \sigma_z^{i_k}}{2} S'(j) S'(k)$$

$$H = \sum_{i,\alpha} h_{\alpha}^i \sigma_{\alpha}^i + \sum_{i,j,\alpha,\beta} h_{\alpha\beta}^{ij} \sigma_{\alpha}^i \sigma_{\beta}^j + \sum_{i,j,k,\alpha,\beta,\gamma} h_{\alpha\beta\gamma}^{ijk} \sigma_{\alpha}^i \sigma_{\beta}^j \sigma_{\gamma}^k + \dots$$

- Reducing the dimensions from  $k$ -local to 2-local by using ancillary qubits
- Illustrative example:

$$\min(\pm x_1 x_2 x_3) = \min(\pm x_4 x_3 + x_1 x_2 - 2x_1 x_4 - 2x_2 x_4 + 3x_4)$$
$$x_1, x_2, x_3, x_4 \in \{0,1\}$$

- This can be used for finding a 2-local representation, yielding the standard Ising Hamiltonian:

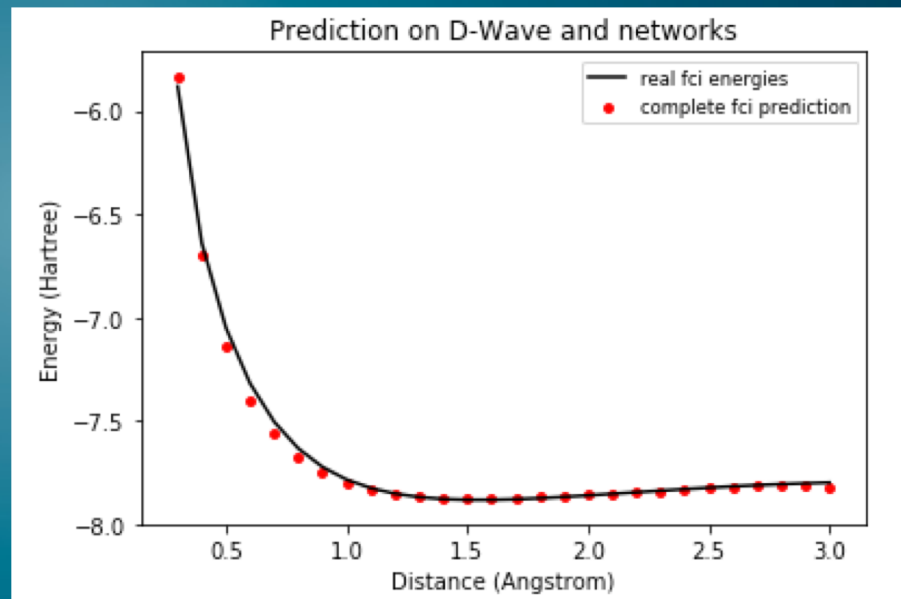
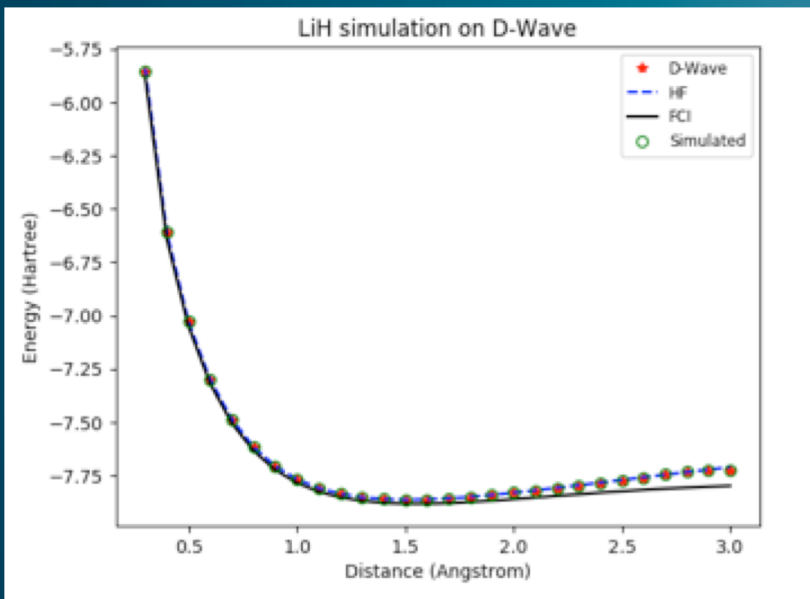
$$H = \sum_i h_i' \sigma_z^i + \sum_{i,j} J_{ij}' \sigma_z^i \sigma_z^j$$



# ELECTRONIC STRUCTURE CALCULATIONS (4)

## Neural network prediction

Sometimes the QPU calculations are a little off





# QUANTUM FINITE ELEMENTS METHOD

## Motivation

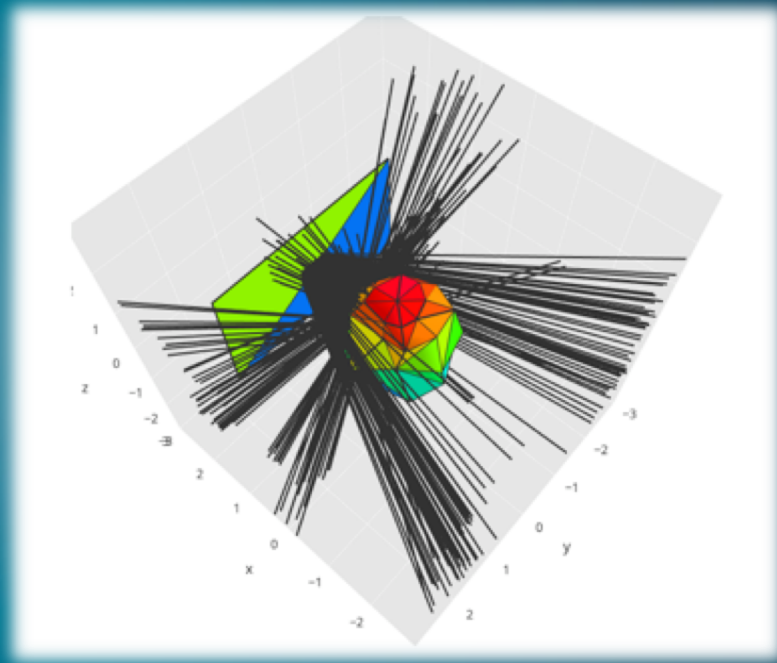
- The finite elements method is used to optimize parts design in order to minimize a quantity, i.e., minimize the sound pressure at a given position around a part, or maximize the durability at certain areas.
- The elements influence each other, so a natural assumption is that qubits connected via couplers can be used to represent it.

## Goal

- Invent a quantum-assisted finite element method for design optimization.

## Actual status and next steps

- First, quantum-assisted finite element method in place
- Application to complex real-world scenarios, i.e., optimization of mirrors or chassis





# QUANTUM-ASSISTED WEIGHT MINIMIZATION FOR VEHICLE CONFIGURATIONS



## Motivation

- CO<sub>2</sub>-calculation is switched from NEFZ to WLTP (individually per vehicle)
- Via the configurator, the customer should be able to calculate CO<sub>2</sub>-span in advance

## Goal

- Minimization of
  - air resistance
  - weight
  - rolling friction

## First results and next steps

- We can both find the minimum and >1 equivalent configuration in the first tests

### Buildability rule:

```
0181900 +MU27 ZMH9Y
X9XAA5G +F EC +FG2 +MA8M +M5TM ZM5T1 /M5TJ
X9XAA33 +ME2N ZMC1Y /MC9C /MU75 /MU76 /M41E /M43A
X9XAA5F +F EC +FG2 +MA8M VM5TM
...
```

### Weights:

UP! 1,0 take 44	(1222A1):	868.0kg
Leichtmetallräder „woodstock“	(43A):	9.64kg
Sitzbezüge in Lederoptik	(N3P):	0.38kg
Sitzbezüge in Stoff	(N2T):	-0.378kg
...		





# QUANTUM-ASSISTED REGRESSION

## Goal

- Optimize the price for vehicles based on changing data sets
- Invent a quantum-enhanced algorithm that does the job

## Motivation

- No one did it before, so we need proof it works
- Our solution generalizes to far more complex machine learning problems, i.e. financial market prediction

## First results and next steps

- Solution quality is equivalent to the best classical algorithms
- Proceed with far more complex problems

Choose yearOfRegistration

Divide it into two parts: older than 14 years- yes =1, no = 0

```
age = []
for a in df['yearOfRegistration']:
    if (a < 2002):
        age.append(1)
    else:
        age.append(0)
df['olderThan14']=age
df.drop('yearOfRegistration', axis=1, inplace=True)
df.head()
```

Unnamed: 0	price	powerPS	kilometer	limousine	kombi	kleinwagen	suv	coupe	cabrio	...	gearbox_notdeclared	...	
0	0	18300	190	125000	0	0	0	0	1	0	...	0	0
1	1	3450	88	100000	0	0	1	0	0	0	...	0	0
2	2	950	114	150000	0	0	0	0	0	0	...	0	0
3	3	10300	170	125000	0	1	0	0	0	0	...	0	0
4	4	8500	193	100000	0	0	0	0	0	0	...	0	0

0 rows x 25 columns

Choose powerPS ranges

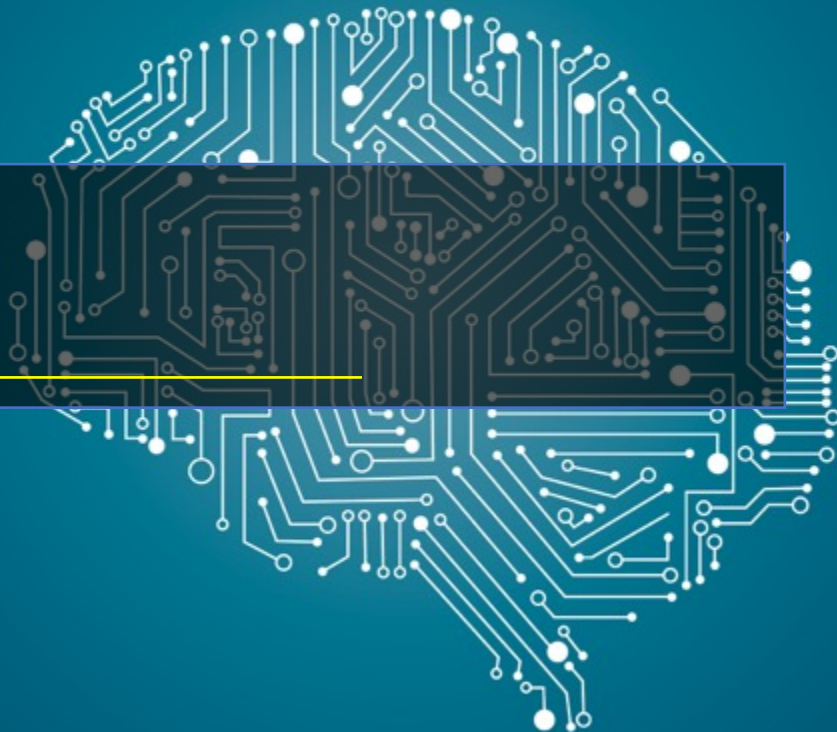
5 ranges 100 steps

```
00a100 = []
0100a200 = []
0200a300 = []
0300a400 = []
0400a500 = []

for p in df['powerPS']:
```

**What's next?**

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# VISION – FURTHER RESEARCH DIRECTIONS

## Quantum machine learning

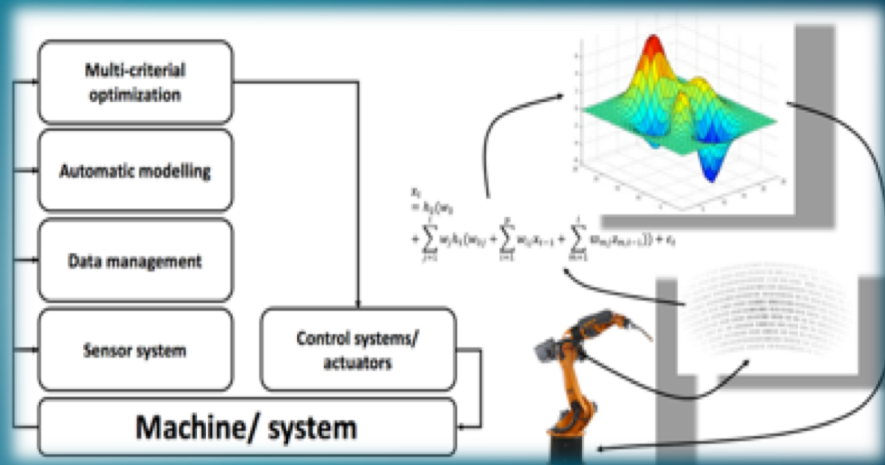
- Grover for ANN function evaluation
- Mapping ANNs directly on the chip
- Graph-splitting in terms of ANNs
- Stacking quantum RBMs to a deep belief net?
- Sampling weight space of ANNs
- Sampling for policy/ value evaluation in reinforcement learning
- Most efficient methods splitting classical and quantum ML
- Linear algebra simulation, i.e. least-squares linear regression

## Quantum simulation

- Materials simulation, i.e. optimized anode or cathode-structure in terms of morphology, composition and doping
- High-temperature superconductivity

## Quantum optimization

- Time-critical optimization problems, i.e. traffic flow
- Optimization of materials, robot behavior





# VISION – SPECIFIC USE CASES (1)

## Materials research

- Materials simulation and optimization, i.e. optimized anode or cathode-structure in terms of morphology, composition and doping
- High-temperature superconductivity simulation – relevant for superconducting electric machines

## Robotics and industry

- Optimization of production processes, faster product customization, variable speed & flexible manufacturing.

- Process optimization and –innovation.
- Optimizing analytics in order to optimize chassis production, corrosion protection, and painting, powertrain, end montage etc.
- Improve current and future operations as well as production (optimization of simulation related to physical processes such as mechanics, fluid dynamics, acoustics, ..., finite element models).
- Response surface mining
- Grid control - optimization of energy distribution





# VISION – SPECIFIC USE CASES (2)

## Enterprise functions optimization

- Optimization of existing multi-variate and time-critical financial analyses and predictions, i.e.
- Financial planning
- Sales and marketing planning
- Product complexity management
- Supply chain and purchasing optimization

## Optimization of complex financial processes, i.e. transaction costs problem:

- Investment with transaction costs
- Asset allocation with transaction costs

- Minimize costs in various areas
- Build portfolios to maximize returns (given a level of risk)
- Maximize efficiency in design and operations of production planning

## Mobility

- Traffic flow under consideration of additional optimization targets (charging pillars, emission reduction, reduction of accidents)
- State space estimation, value iteration, and finding the optimal policy in a given state (quantum reinforcement learning).



# WE CHALLENGE QC, TOO

## Implemented Algorithms:

- Simulated Annealing
- Parallel Tempering
- Markov Logic Network
- Mixed Integer Linear Program
- Greedy Optimisation
- tbd.

## Implemented calls to ext. solvers:

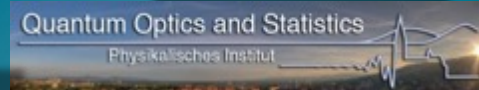
- Qbsolve (D-Wave)
- Toulbar2 (INRA)
- CPLEX (IBM)
- tbd.

```
11 Logger.getLogger("org.drosophila.jqf.jqf.ParallelTempering");
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21 * Implementation of parallel tempering. This is an extension of simulated annealing
22 * where several chains run in parallel, each at a different temperature.
23 * Neighbouring chains can periodically swap their states, where the probability of
24 * a swap depends on the energy difference and the temperature difference.
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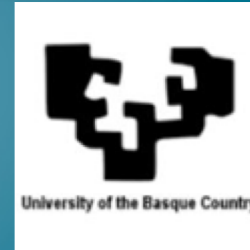
The API will be **made available** to the **Volkswagen Group** during the next months and is planned to be put open source later



# RESEARCH AND EXCHANGE WITH



- Partnerships for grant proposals with FZ Juelich, Siemens, DLR, Trumpf
- 5 university partnerships, 9 research contracts
- Quantum Annealing (QA) and Machine Learning (RBMs, HQMMs, Q-Bayes-Nets, etc.)
- Risk and Quality-of-Service with QA: Analysis of the result distribution
- Quantum/classic-hybrid: Analysis of sequential Entscheidungsprobleme
- Analysis of the construction of optimisation problems for QA
- Porting a C/C++/Python/Shell-Library into a Java-API + Best Practices
- Relationship between Annealing time and result quality
- Influence of choice of final state used on the result quality
- Relationship between good/best solution, number of queries and problem size
- Effects on the anneal time via quantum simulation
- Potential partnership with Los Alamos National Lab





Material Simulation >

# THANK YOU

< Battery Optimization