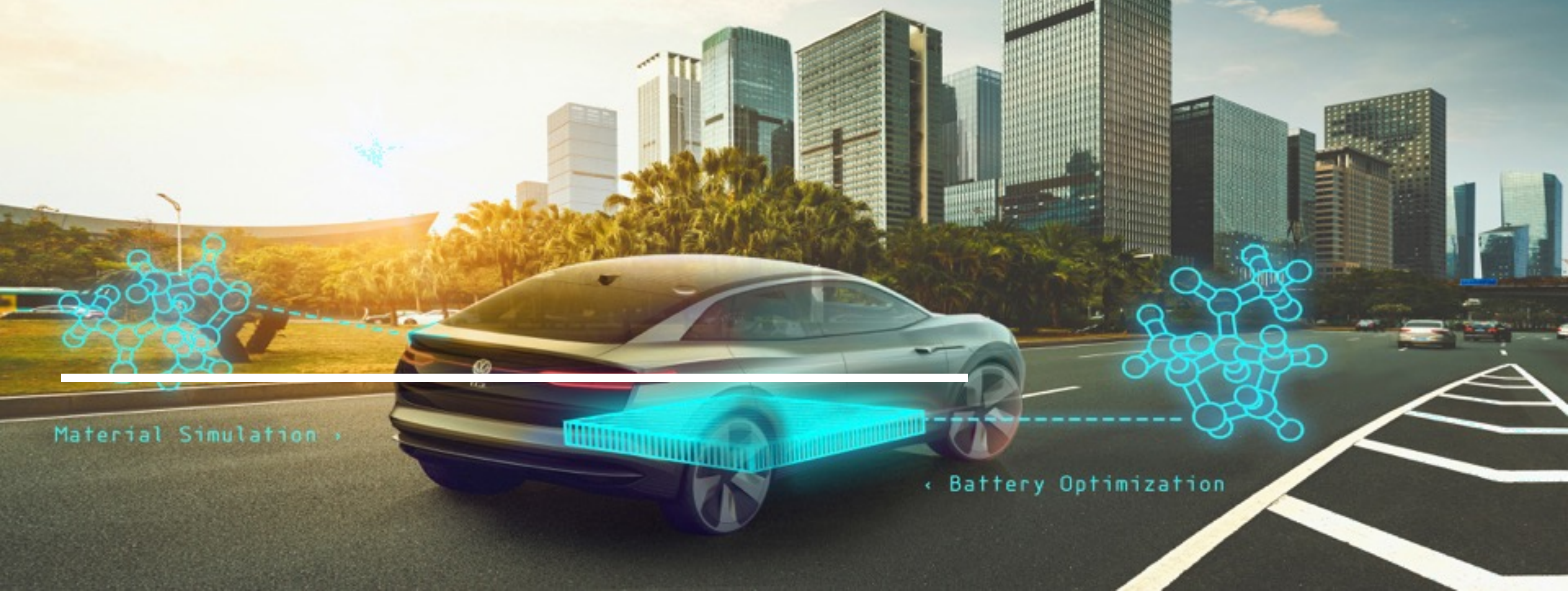
Near-term QC applications in industry

Florian Neukart

Volkswagen Group, Region Americas



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:

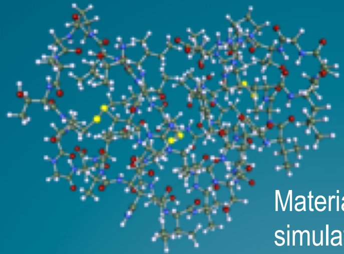
- Quantum-assisted machine learning
- Augmentation of deep learning, reinforcement learning, optimization algorithms and sampling
- Quantum simulation

		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)

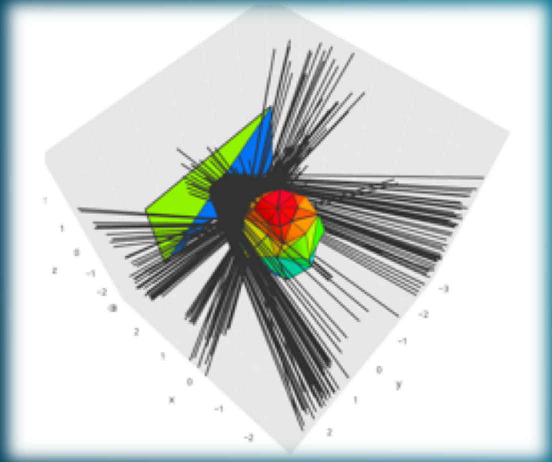
With classical computers, many of the most complex problems can’t be solved.



Materials simulation

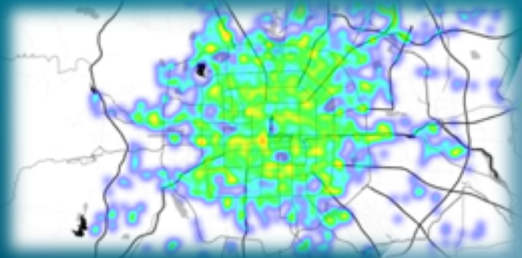
Quantum annealing – some things we’ve done so far

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

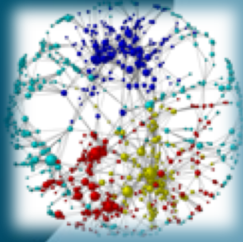


Finite elements design

Traffic flow optimization



Reinforcement learning

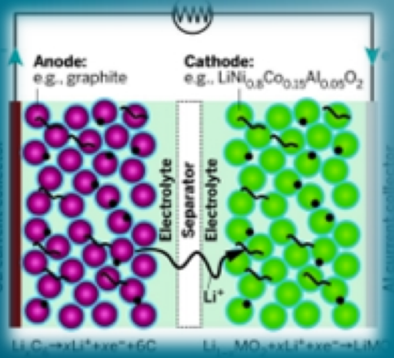


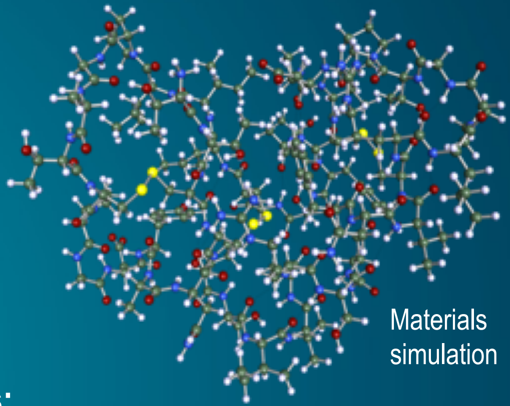
Clustering

WHAT'S HAPPENING AT VW (2)

Gate model – we are working on

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





Materials simulation

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

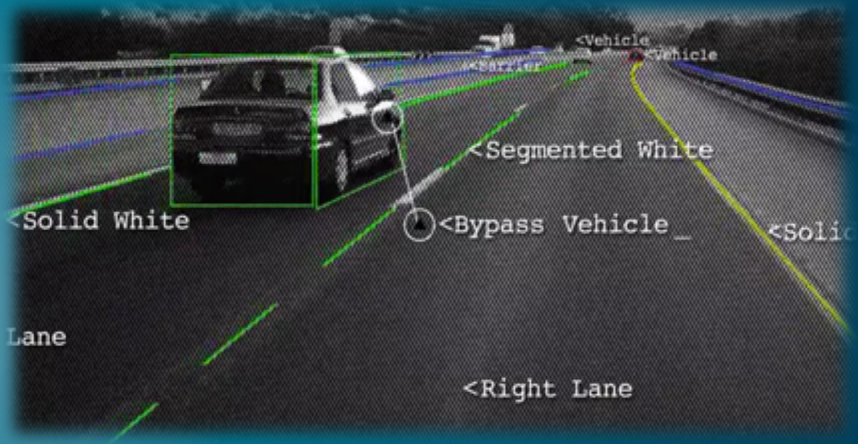
- Rewarding good results, i.e., simulating millions of parking maneuvers and rewarding successful ones.
- Agents, such as self-driving vehicles, intend to find the best thing to do in a given situation to reach their goal (parking, maneuvering through traffic, etc.) – they learn by trial and error.

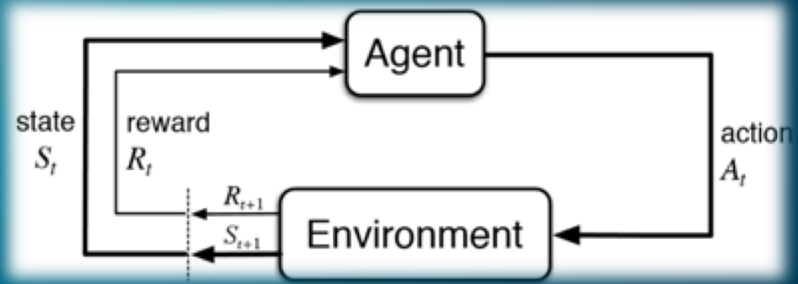
Goal: the closer to the real-world simulations are, the better the results

- 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

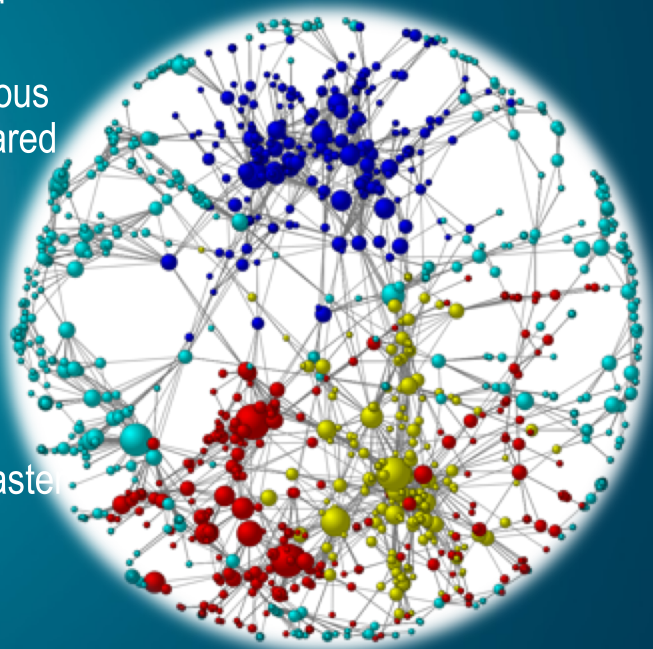
- Clustering is useful in a variety of applications, especially for uncovering and understanding network behavior, i.e.:
  - model how something can move through a network. For example, malicious software will propagate more quickly through a dense community, compared to a sparse one
  - extrapolate 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

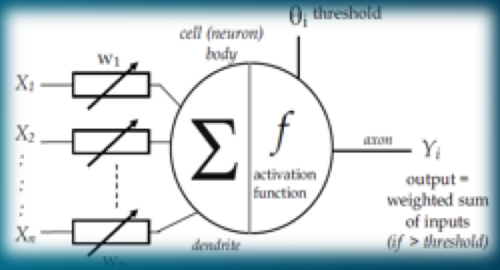
- Artificial neural networks may be used whenever software cannot be explicitly programmed to solve a task (or only with significant effort).
- Optimize a performance criterion using example data or past experience.

Goal

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

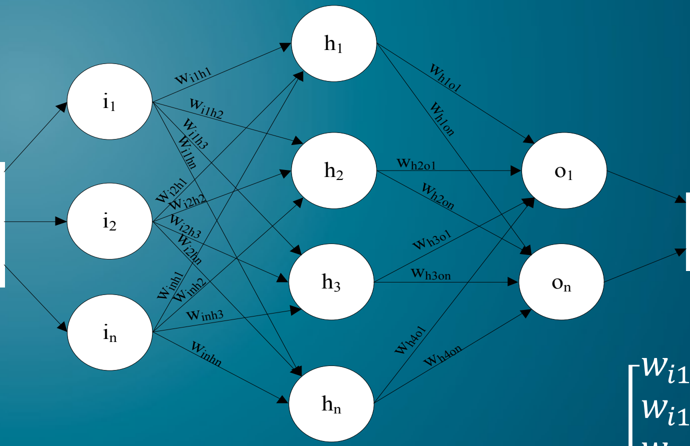
Actual status

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



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

$$v_i = \begin{bmatrix} x_1 \\ x_2 \\ x_n \end{bmatrix}$$



$$\begin{bmatrix} x_1 \\ x_n \end{bmatrix} = v_o$$

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

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

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 weightspace.
- 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

$$Xw = \hat{y}$$

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

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

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

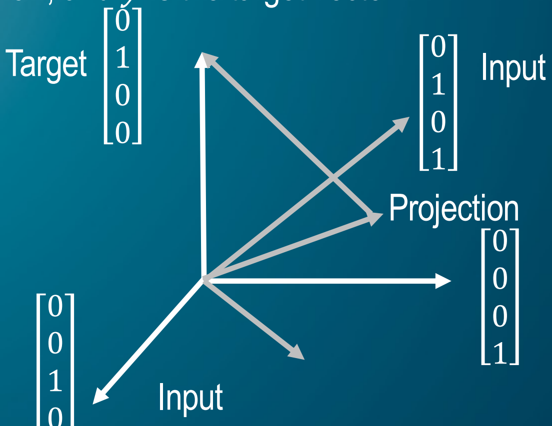
$$\arg\min_w Q\hat{y}$$

A very, very simple example

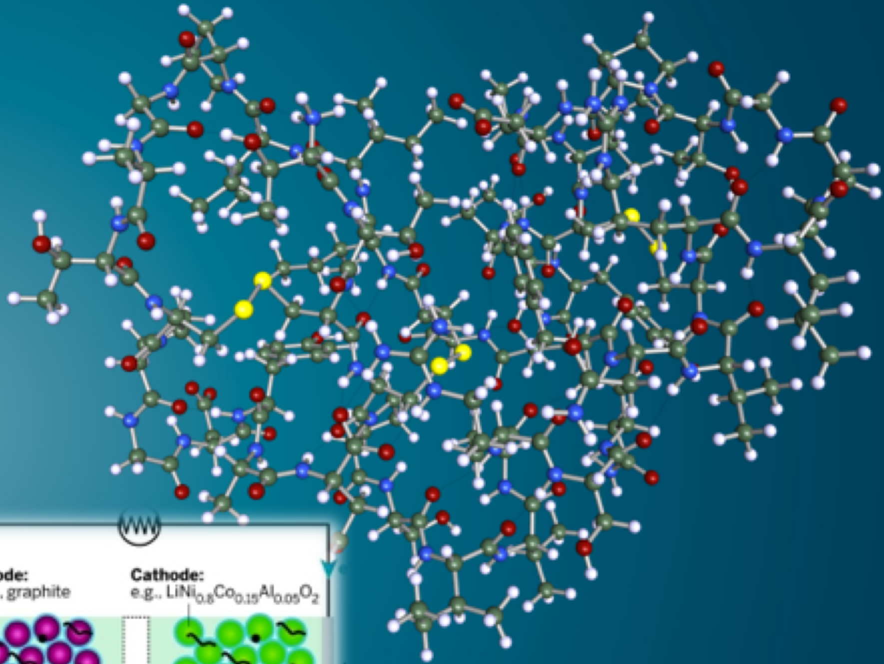
$$Xw = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} 0 \\ w_1 \\ w_2 \\ w_1 w_2 \end{bmatrix} = \hat{y}$$

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.

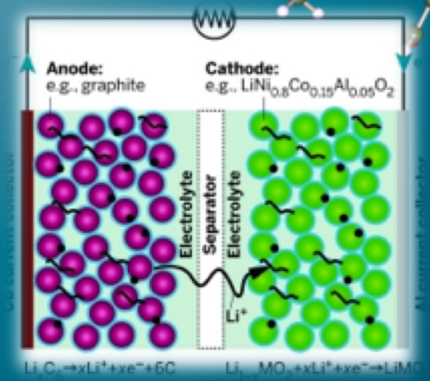


ELECTRONIC STRUCTURE CALCULATIONS (1)



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)

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

ELECTRONIC STRUCTURE CALCULATIONS (3)

- Hamiltonian consisting of qubit operators only, but how to map it on a QUBO?
  - σ_x, σ_y and σ_z terms instead of σ_z terms only
  - k-local terms instead of 2-local
- Below we show how to map such a n-qubit Hamiltonian with σ_x, σ_y and σ_z terms to a rn-qubit Hamiltonian with σ_z terms only

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

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

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

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

$$\min(\pm x_1 x_2 x_3) = \min(\pm x_4 x_3 + x_1 x_2 - 2x_1 x_4 - 2x_2 x_4 + 3x_4)$$

$$x_1, x_2, x_3 x_4 \in \{0,1\}$$

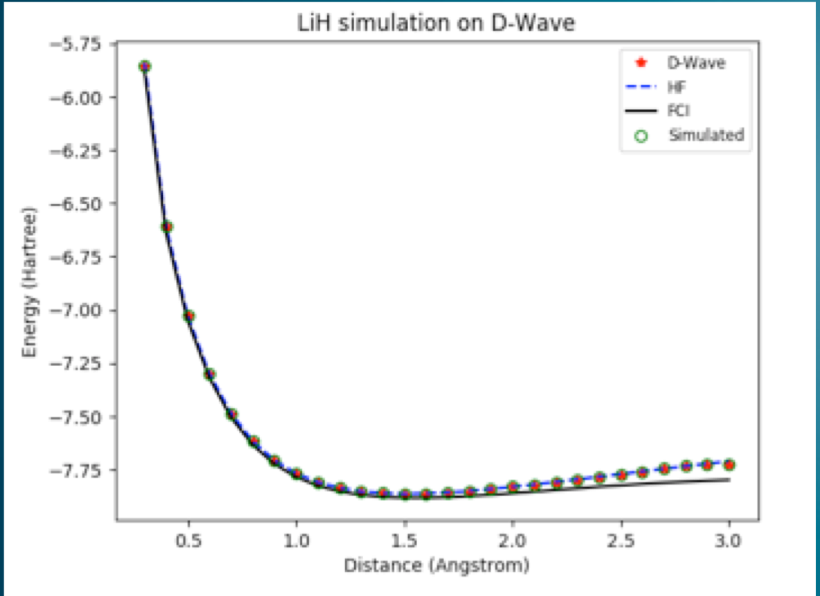
- This can be used for finding a 2-local representation, yielding the standard Ising Hamiltonian:

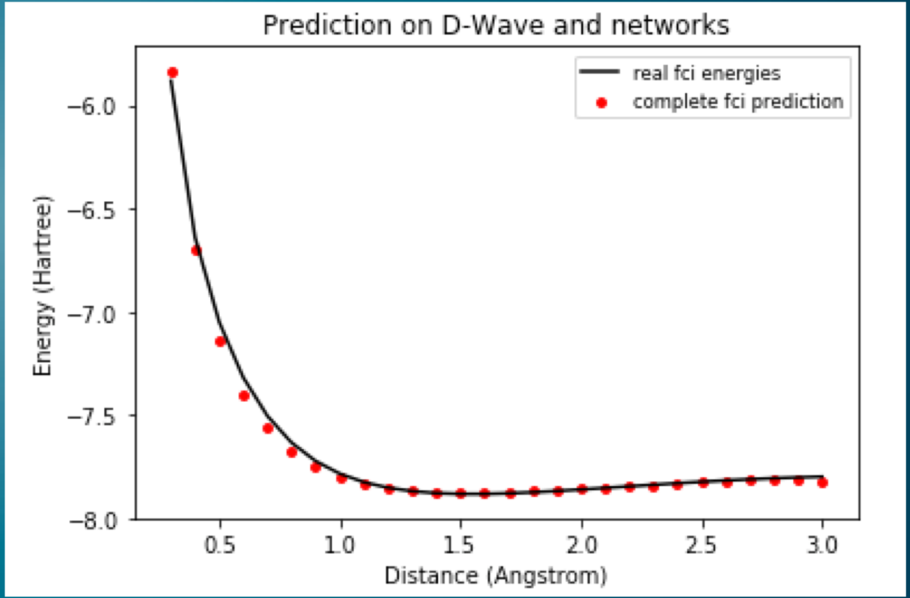
$$H = \sum_i h_i' \sigma_z^i + \sum_{i,j} J_{ij}' \sigma_z^i \sigma_z^j$$

ELECTRONIC STRUCTURE CALCULATIONS (4)

Neural network prediction

Sometimes the QPU calculations are a little off





QUANTUM FINITE ELEMENTS METHOD

Motivation

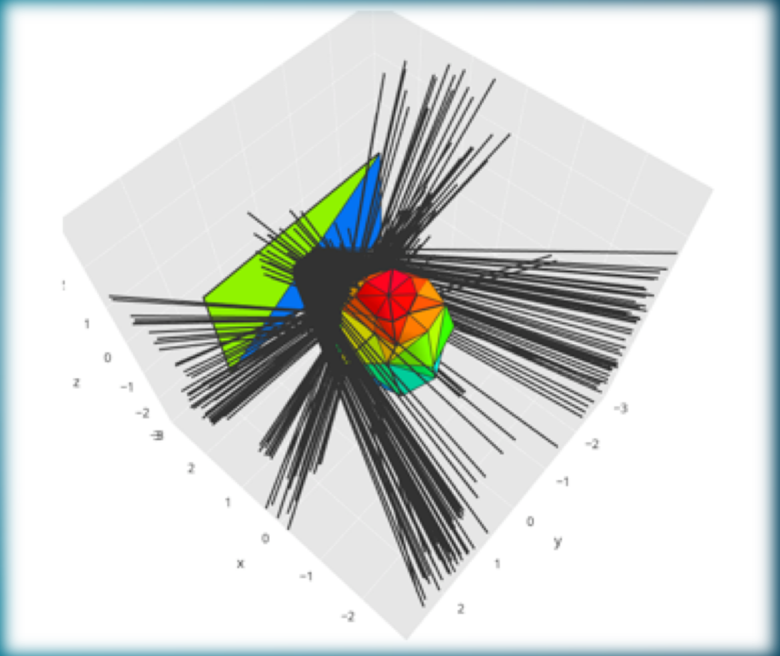
- The finite elements method is used to optimize parts design in order to minimize a quantity, i.e., minimize the sound pressure at a given position around a part, or maximize the durability at certain areas.
- The elements influence each other, so a natural assumption is that qubits connected via couplers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

OPERATIONS.RESEARCH:LAB
WOLFSBURG

Motivation

- CO_2–calculation is switched from NEFZ to WLTP (individually per vehicle)
- Via the configurator, the customer should be able to calculate CO_2-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

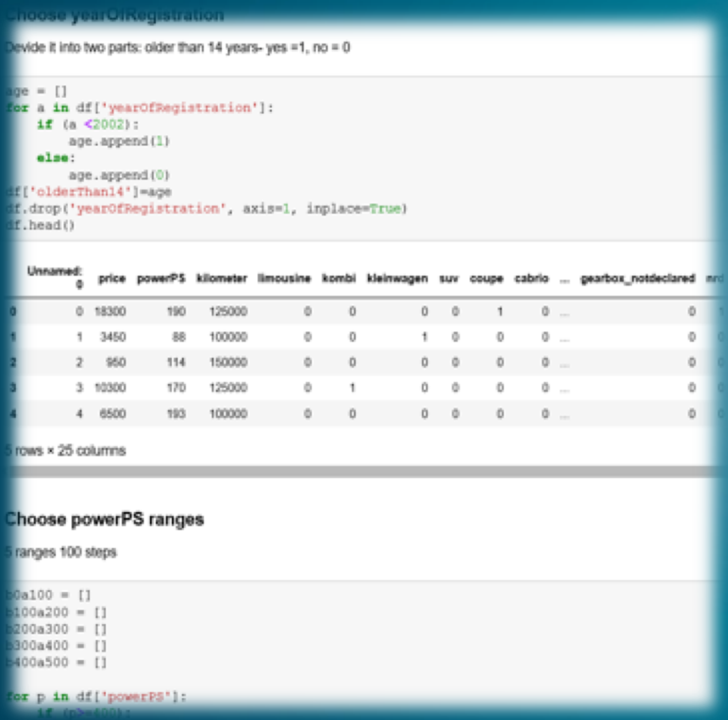
Buildability rule:

0181900 +MU27 ZMH9Y
X9XAA5G +F EC +FG2 +MA8M +M5TM ZM5TI /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



Choose yearOfRegistration

Devide 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
1	1	3450	88	100000	0	0	1	0	0	0	...	0
2	2	950	114	150000	0	0	0	0	0	0	...	0
3	3	10300	170	125000	0	1	0	0	0	0	...	0
4	4	6500	193	100000	0	0	0	0	0	0	...	0

5 rows × 25 columns

Choose powerPS ranges

5 ranges 100 steps

```
b0a100 = []
b100a200 = []
b200a300 = []
b300a400 = []
b400a500 = []

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

Goal

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

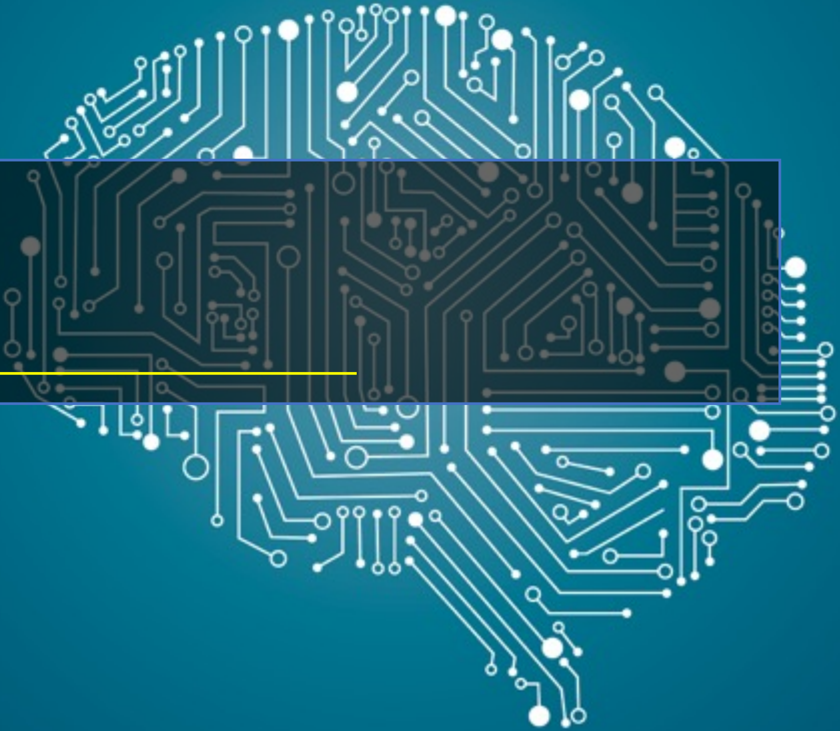
Motivation

- 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

What’s next?



VISION – FURTHER RESEARCH DIRECTIONS

Quantum machine learning

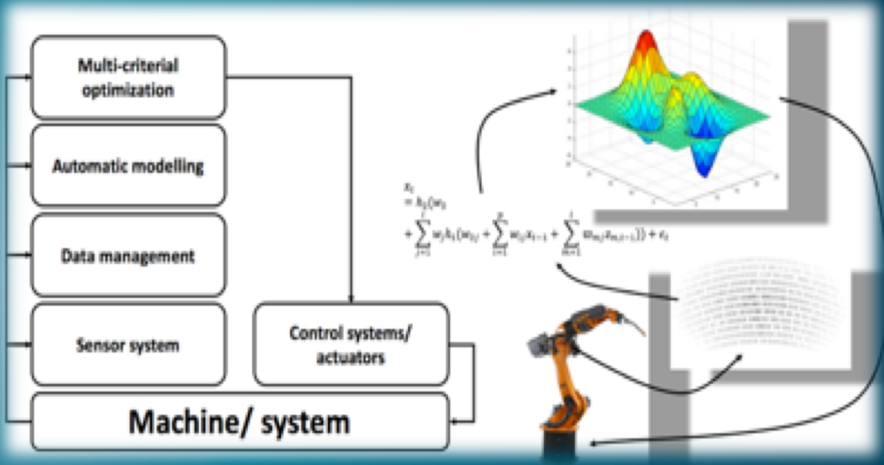
- Grover for ANN function evaluation
- Mapping ANNs directly on the chip
- Graph-splitting in terms of ANNs
- Stacking quantum RMBs to a deep belief net?
- Sampling weight space of ANNs
- Sampling for policy/ value evaluation in reinforcement learning
- Most efficient methods splitting classical and 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).

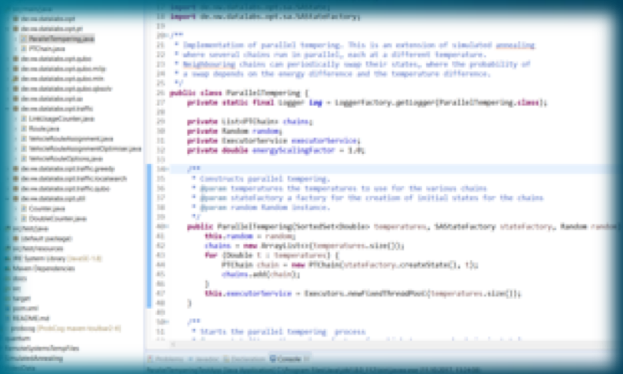
WE CHALLENGE QC, TOO

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.



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 Entscheidungsproblems
  - 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**

Leiden Institute of Advanced Computer Science

THANK YOU