

Quantum Computing for Computational Engineering

JARA CSD Panel Discussion



Forschungszentrum

Quantensprung: Start für neuen Computer in Jülich

Aktualisiert am 18. Januar 2022

QUANTENTECHNOLOGIE ZUM TESTEN Quantensprung in Jülich

VON MANFRED LINDINGER · AKTUALISIERT AM 17.01.2022 · 21:03

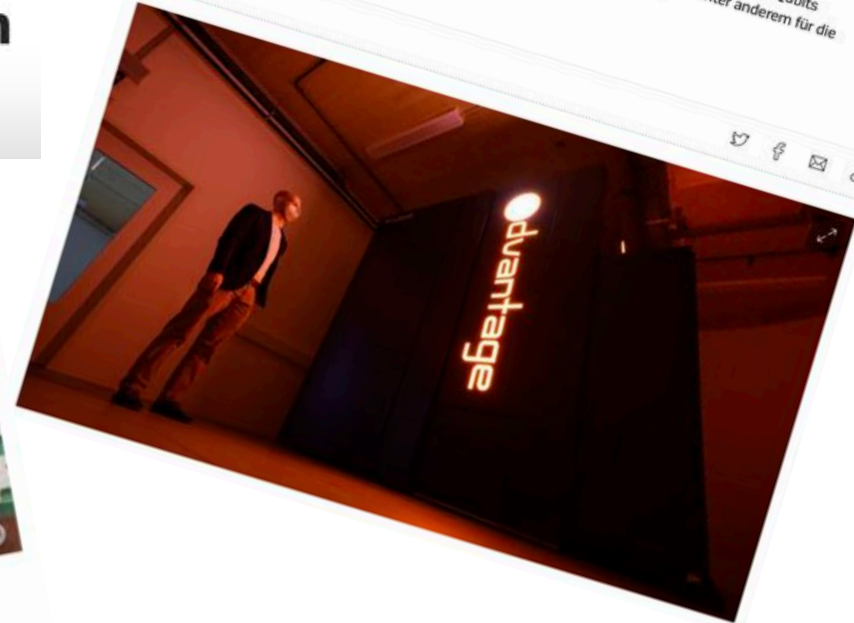


Am Forschungszentrum Jülich steht seit Montag dieser Woche ein kommerzieller Quantenrechner. Es ist ein Rechner der kanadischen Firma D-Wave mit 5000 Quantenbits. Die leistungsfähige Maschine soll vor allem komplexe Optimierungsaufgaben lösen.

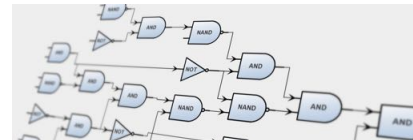
Neuer Supercomputer in Betrieb Quantensprung in Jülich

Am Forschungszentrum Jülich ist der erste Quantencomputer mit mehr als 5000 Qubits außerhalb Nordamerikas in Betrieb. Die komplexe Rechenleistung soll unter anderem für die Klimaforschung genutzt werden.

17.01.2022, 17:05 Uhr



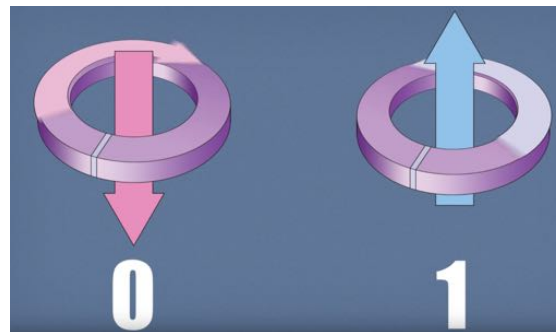
- Quantum leap:
- a) Revolution of computing?
- b) Smallest possible step in nature?



The quantum computing mystery

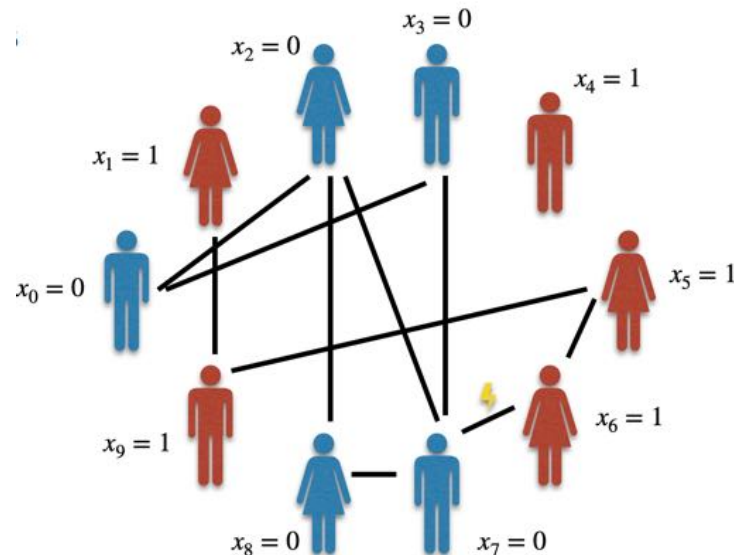
- **Classical computing:** Data stored & processed in **bits**, which are either 0 or 1
- **Quantum computing:** **Qubits** store also superposition states; quantum parallelism treats all states simultaneously

$$\frac{1}{\sqrt{2}}|\text{cat}\rangle + \frac{1}{\sqrt{2}}|\text{dog}\rangle$$



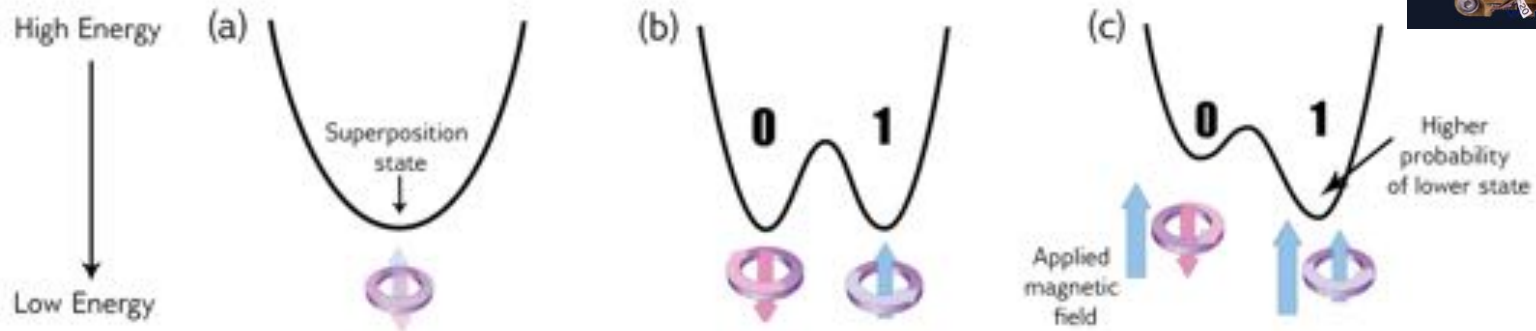
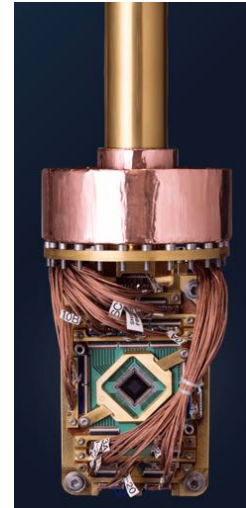
Quantum annealing

- The D-Wave quantum annealer is not a general purpose quantum computer
- It can solve certain discrete optimisation problems



Quantum annealing

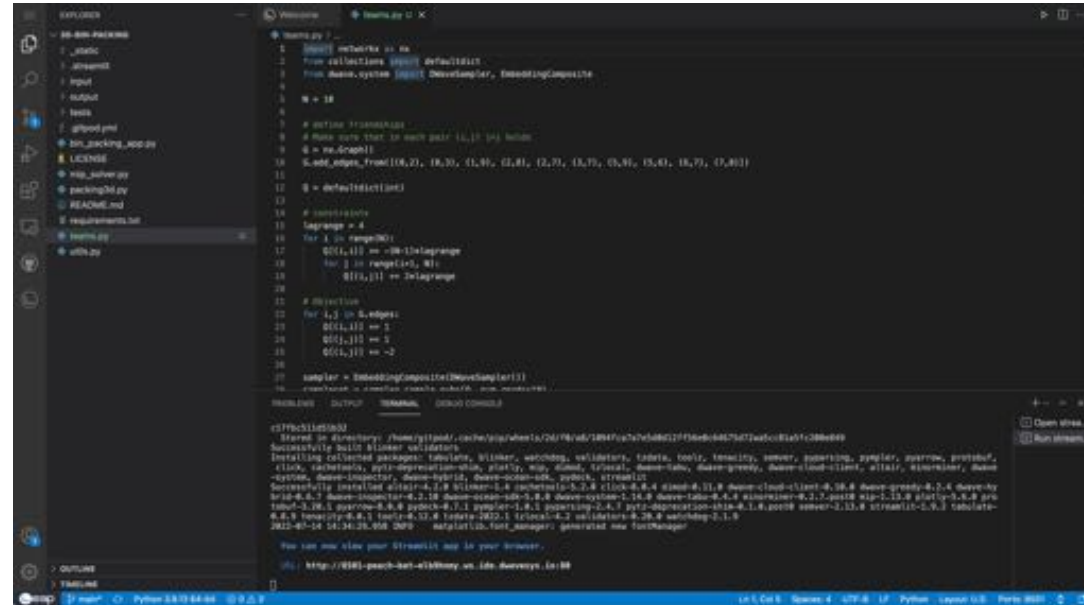
- With **quantum annealers** you initialise the system in a low-energy state and gradually introduce the parameters of a “task” you wish to optimise.
- The Quantum Processing Unit operates at temperatures below 15 mK, and need to be shielded from electromagnetic waves



QUBO

- QUBO formulation as upper triangular $N \times N$ matrix Q . Minimize

$$E(\{x_i\}) = \sum_i Q_{ii}x_i + \sum_{i < j} Q_{ij}x_i x_j$$



```

1 # imports
2 from collections import defaultdict
3 from math import sqrt, floor, ceil
4
5 N = 10
6
7 # define the graph
8 # Make sure that in each pair (i,j) both
9
10 G = nx.Graph()
11 G.add_edges_from([(0,2), (0,3), (1,0), (2,0), (2,7), (3,7), (3,9), (5,0), (6,7), (7,0)])
12
13 Q = defaultdict(int)
14
15 # coefficients
16 lagrange = 4
17 for i in range(N):
18     Q[i,i] += -10*lagrange
19     for j in range(i+1, N):
20         Q[i,j] += 2*lagrange
21
22 # objective
23 for i,j in G.edges:
24     Q[i,j] += 1
25     Q[j,i] += 1
26     Q[i,i] += -2
27
28 solver = EmbeddingComposite(DWaveSampler())
29
30
31

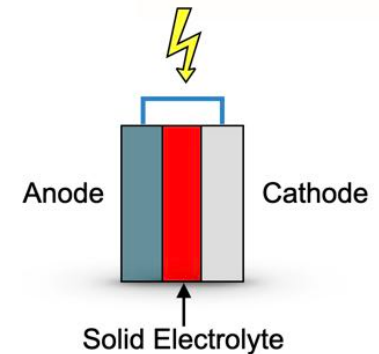
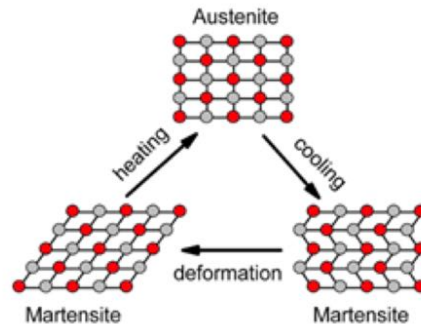
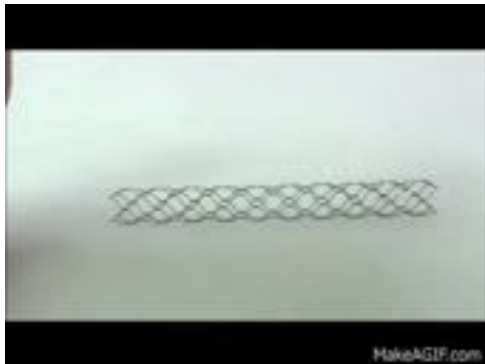
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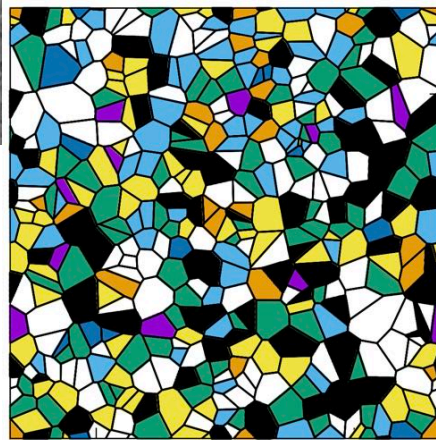
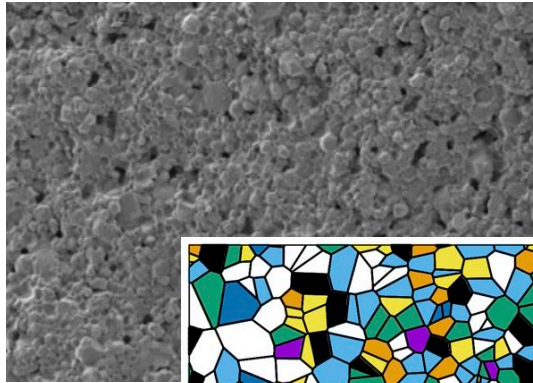
Leap IDE /workspace/3d-bin-packing $ cd /workspace/3d-bin-packing
Files/lib/python/debugpy/launcher 43861 -- /workspace/3d-bin-packing
0 0 1 2 3 4 5 6 7 8 9 energy num_oc. chain_
1 0 1 0 1 1 0 0 0 1 1 0 -99.0 4 0.0
2 1 1 0 0 1 1 1 0 0 0 1 -99.0 4 0.0
3 0 0 1 0 0 1 1 1 1 0 0 -97.0 2 0.0
4 0 0 1 0 1 0 1 1 1 0 0 -97.0 1 0.0
5 0 0 1 1 0 0 1 1 1 0 0 -97.0 1 0.0
6 0 1 0 1 0 1 1 1 0 0 1 -97.0 1 0.0
7 0 1 0 0 0 1 1 1 0 0 1 -97.0 2 0.0
8 1 1 0 0 0 1 1 0 0 1 -97.0 2 0.0
9 0 1 0 0 0 1 1 0 1 1 -97.0 2 0.0

```


Quantum annealing for materials science



Quantum annealing for microstructures



Step 1: Compute grain-grain interactions (classical)

Step 2: Find optimal variant distribution (quantum)

