UNIVERSITÄT PADERBORN
Die Universität der Informationsgesellschaft

Introduction to Quantum Computing

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Paderborn Center for Parallel Computing

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Introduction to Quantum Computing

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1. Qubits, States and Complexity
2. Challenges in Practice
3. An Interesting Algorithm for an HPC Workload
4. Outlook

Introduction to Quantum Computing

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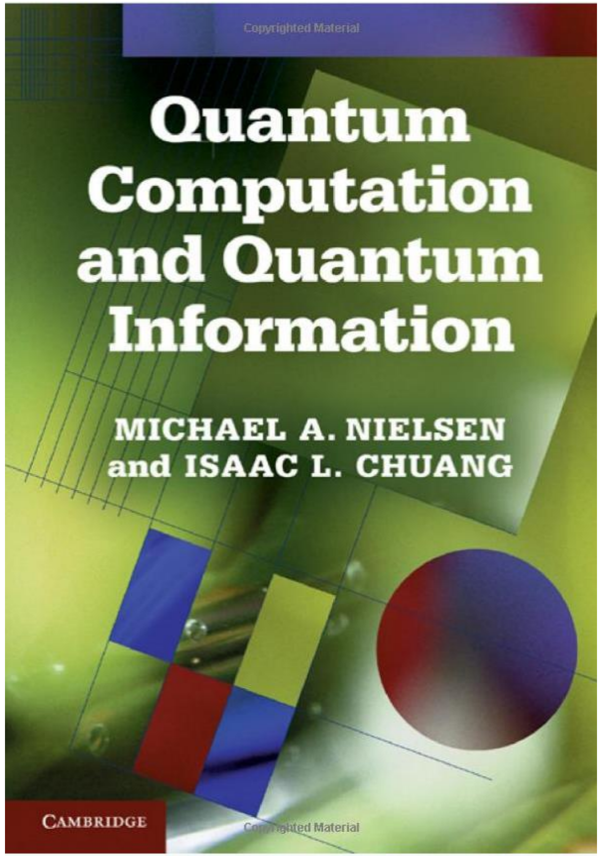
Disclaimers:

- I'm a **theoretical** physicist/chemist, so not a lot about experiments.
- This talk is very short, I had to throw in many grains of salt!
- This talk is focussed on **gate-based quantum computers** (Google, IBM,… but not D-Wave).
- **Great book**: Quantum Computation and Quantum Information, (Nielsen and Chuang)
- Experiments with QC:
    - https://quantum-computing.ibm.com/



Why Quantum Computers?

No efficient classical algorithms are known for many problems:

Factoring numbers:

3 x 7

=

21

Multiplication: simple

Factorization in prime numbers: still simple (for small numbers)

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Why Quantum Computers?

No efficient classical algorithms are known for many problems:

Factoring numbers:

Multiplication: simple
1 ms on a single cpu-core

3347807169895689878604416984821269081770479498371376856891243138898288379387800228761471165253174308773781446799948
9
x
36746043666799590428244633799627952632279158164343087642676032283815739666511279233373417143396810270092798736308917

=

12301866845301177551304949583849627207728535695953347921973224521517264005072636575187452021997864693899564749427740638459251925573263034537315482685079170261221429134616704292143116022212404792747377940806653514195974598569021434 13

$\in \mathcal{O}(2^k)$

Factorization in prime numbers:
HARD on classical computers!!!

768-bit RSA:

"2000 years of computing on a single-core 2.2 GHz AMD Opteron-based computer"

(https://eprint.iacr.org/2010/006.pdf)

- **BUT**: there is an **efficient <u>quantum</u> algorithm** to factor numbers:
  Shor's Algorithm by Peter Shor (*SIAM J. Comput.*, 26(5), 1484–1509., 1994)
  Complexity: $\in \mathcal{O}(k^3)$

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Why Quantum Computers?

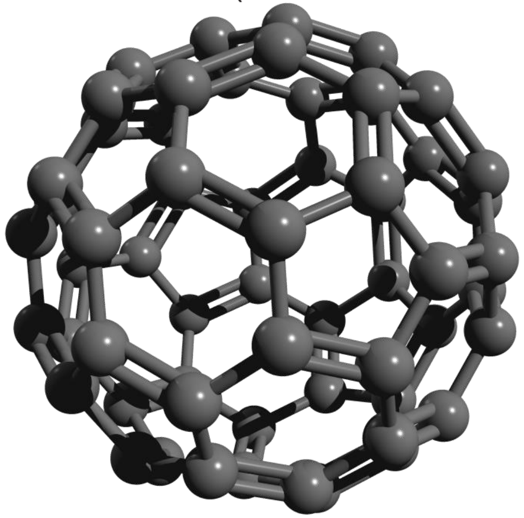
No efficient classical algorithms are known for many problems:

Quantum Chemistry, Solid-State Physics,…:

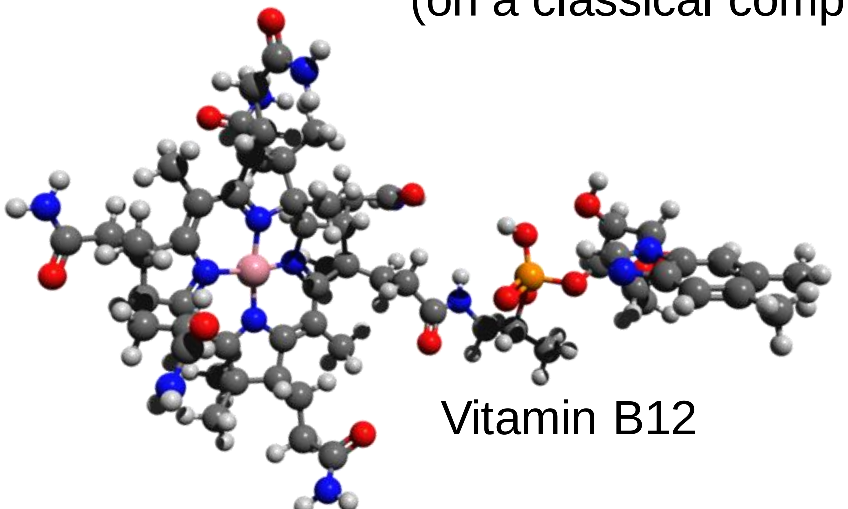
Challenge is to describe **quantum** systems (atoms, molecules, ...) on **classical** computers.

$$\left(\sum_i \frac{\hat{p}_i^2}{2m_e} + \sum_A \frac{\hat{P}_A^2}{2M_A} + \frac{1}{2}\sum_{i\neq j} \frac{e^2}{4\pi\epsilon_0 |\hat{r}_i - \hat{r}_j|} + \frac{1}{2}\sum_{A\neq B} \frac{e^2 Z_A Z_B}{4\pi\epsilon_0 |\hat{R}_A - \hat{R}_B|} - \frac{1}{2}\sum_{A,i} \frac{e^2 Z_A}{4\pi\epsilon_0 |\hat{R}_A - \hat{r}_i|} \right) |\Psi(t)\rangle = i\hbar\partial_t |\Psi(t)\rangle$$

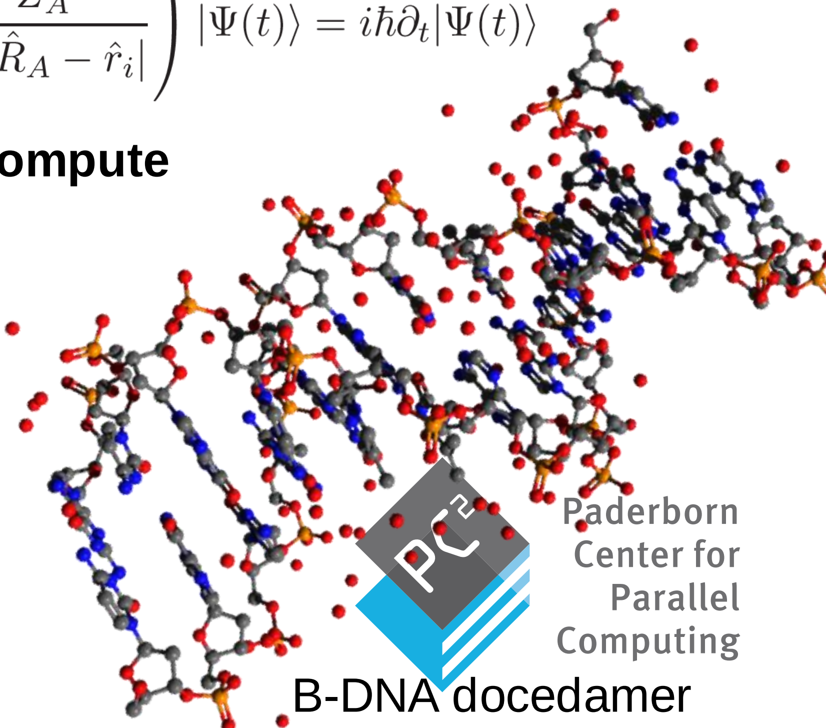
All basic physical laws are known, just **to hard to compute** (on a classical computer).



C60 Fullerene



Vitamin B12



B-DNA docedamer

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Qubits, States and Complexity

Classical computer

Storage unit:

Bit

S=|0⟩ OR S=|1⟩

Qubits, States and Complexity

Classical computer

Storage unit:

Bit

$S=|0\rangle$ OR $S=|1\rangle$

Quantum computer

Storage unit:

Qubit

$S=|0\rangle$ $S=|1\rangle$

$$\mathbf{S=a|0\rangle+ b|1\rangle}$$

(a,b complex numbers, $1=a^2+b^2$)

A quantum system can be in **more than one** state at a time:
Superposition

$S=|0\rangle + |1\rangle$:

- system is 50% in state $|0\rangle$ and 50% in state $|1\rangle$
  at the same time!

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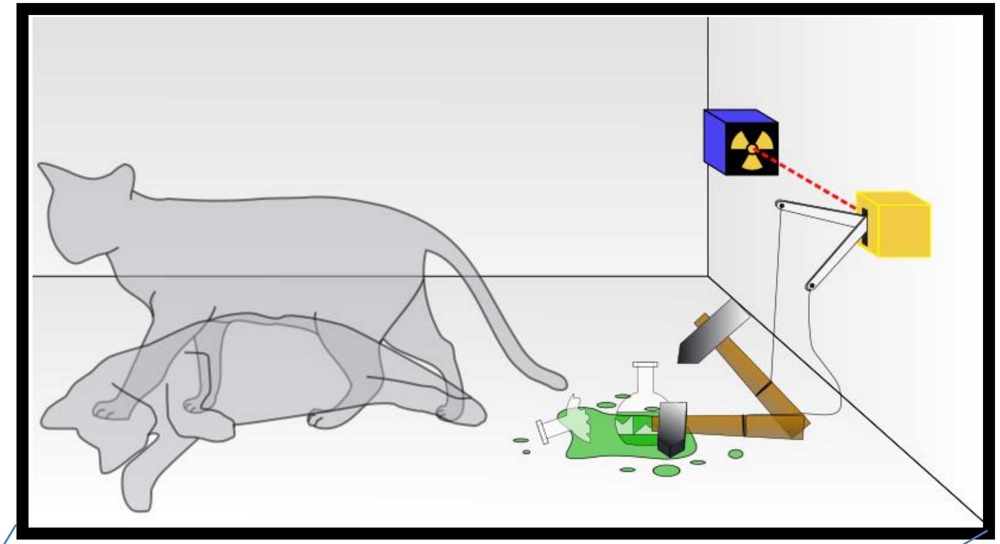
Superposition

Sketch by Dhatfield
(https://commons.wikimedia.org/wiki/File:Schrodingers_cat.svg)



S=|0⟩ + |1⟩:

- system is 50% in state |0⟩ and 50% in state |1⟩
  at the same time!

Schrodinger's cat (1935): thought experiment

Imagine a **cat in a closed box** with a poison:

- A random element (e.g. radioactive decay) controls the release of posion

- The cat can be thought of as
  dead |dead⟩ and alive |alive⟩ at the same time!
  S_{cat}=|dead⟩+|alive⟩

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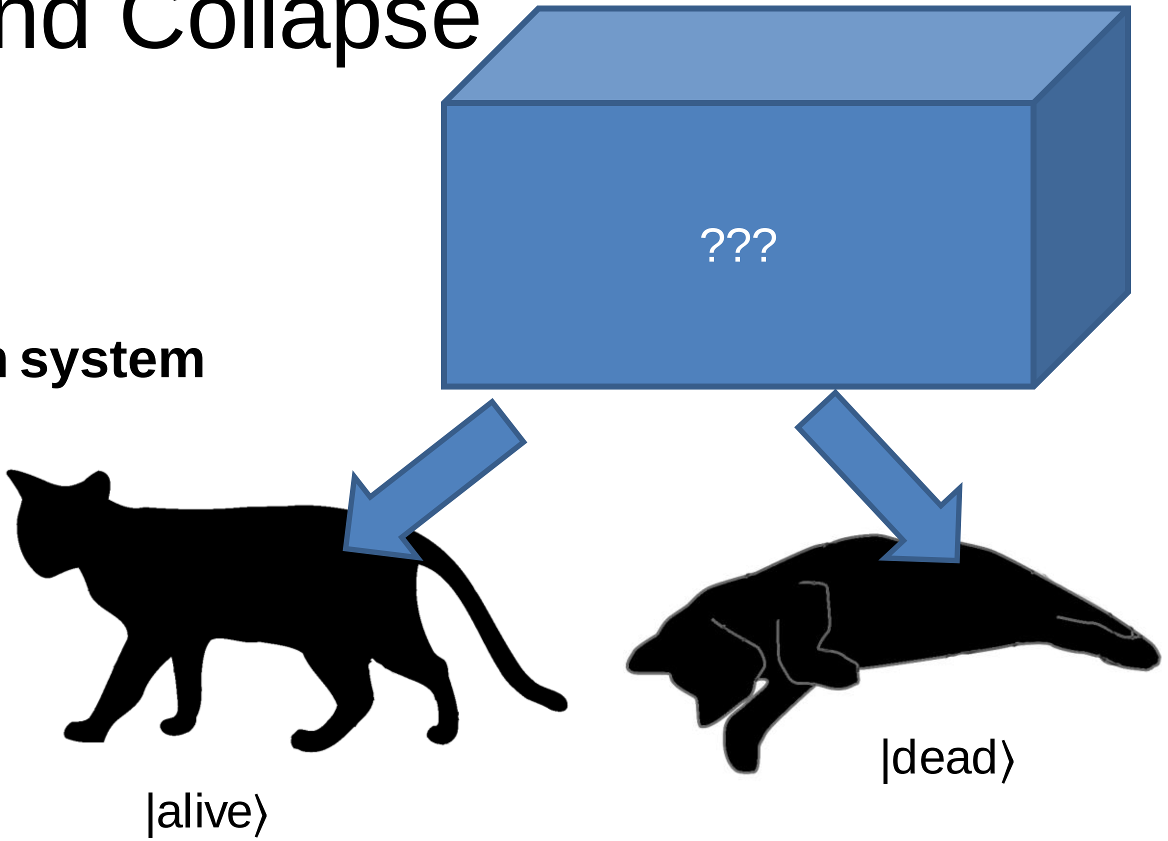
Superposition and Collapse

$S_{cat}=|dead\rangle+|alive\rangle$

- As long as the box is closed, we don't know.
- When we open the box we **disturb the quantum system and the state collapses:**
  quantum-mechanical measurement



- **We measure**
  - with 50% probability |alive>
  - with 50% probability |dead>

(The collapse of the state is nothing magical, but can be described by quantum decoherence of a system (the box) interacting with the environment.)

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Qubits, States and Complexity

<u>Classical computer</u>

Storage unit: **Bit**

$S=|0\rangle$ OR $S=|1\rangle$

Multiple storage units: N=8 bits

$S=|01011010\rangle$="Z"

$2^N=256$ different possibilities

A state is determined by **one integer number**.

Information stored = **N bits**

= 64 bit for N=64

<u>Quantum computer</u>

Qubits, States and Complexity

Classical computer

Storage unit: **Bit**

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Multiple storage units: N=8 bits

S=|01011010⟩="Z"

2^N=256 different possibilities

A state is determined by **one integer number**.

Information stored = **N bits**
= 64 bit for N=64

Quantum computer

Storage unit: **Qubit**

S=|0⟩ S=|1⟩

S=a|0⟩+ b|1⟩

Multiple storage units: N=8 Qubits

$S=a_0|00000000\rangle+a_1|10000000\rangle+a_2|01000000\rangle+a_3|11000000\rangle+\dots$

A state is determined by an **exponential number (2^N) of complex numbers (a_0, a_1,…).**

Information stored = **2^N x 128 bit**
= **295148 PB** for 64 qubits

(assuming 64-bit double precision for the complex numbers)

Qubits, States and Complexity

Operations on quantum states:

S=a|0⟩ + b|1⟩ $\xrightarrow{\text{Op}}$ S'=Op(S)=a'|0⟩ + b'|1⟩

An operation Op maps a,b to a',b'

- Can be written as a **unitary transformation**, i.e., a 2x2 matrix U with $U^{-1}=(U^T)^*$

$$\begin{pmatrix} a' \\ b' \end{pmatrix} = U \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}$$

Unitary ($U^{-1}=(U^T)^*$) because:

- Operation needs to be **reversible**
- Resulting state needs to be **normalized**, i.e. $a^2 + b^2 = 1 \quad \Rightarrow \quad a'^2 + b'^2 = 1$

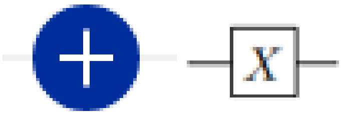
Very general, but hard to understand/imagine the operation.

Qubits, States and Complexity

Operations on quantum states:

Example: x-gate

$$U_\mathrm{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$



$$U_\mathrm{x}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} b \\ a \end{pmatrix} \quad \text{or} \quad U_x(a|0\rangle + b|1\rangle) = a|1\rangle + b|0\rangle$$

x-gate "switches" (flips) the qubit from $|0\rangle$ to $|1\rangle$ and vice versa.

name	unitary matrix	visual representation
Hadamard gate (h)	$\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$	$\lvert q_0\rangle$ H
σ_x gate (x)	$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$	$\lvert q_0\rangle$ X
σ_y gate (y)	$\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$	$\lvert q_0\rangle$ Y
σ_z gate (z)	$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$	$\lvert q_0\rangle$ Z
R_x gate (rx)	$e^{-i\theta\sigma_x/2} = \begin{pmatrix}\cos(\theta/2) & -i\sin(\theta/2)\\ -i\sin(\theta/2) & \cos(\theta/2)\end{pmatrix}$	$\lvert q_0\rangle$ $R_x(\theta)$
R_y gate (ry)	$e^{-i\theta\sigma_y/2} = \begin{pmatrix}\cos(\theta/2) & -\sin(\theta/2)\\ \sin(\theta/2) & \cos(\theta/2)\end{pmatrix}$	$\lvert q_0\rangle$ $R_y(\theta)$
R_z gate (rz)	$e^{-i\theta\sigma_z/2} = \begin{pmatrix}e^{-i\theta/2} & 0\\ 0 & e^{i\theta/2}\end{pmatrix}$	$\lvert q_0\rangle$ $R_z(\theta)$
phase shift	$e^{i\theta\mathbb{1}} = \begin{pmatrix}e^{i\theta} & 0\\ 0 & e^{i\theta}\end{pmatrix}$	$\lvert q_0\rangle$ $Ph(\theta)$
rotation gate (u3)	$\begin{pmatrix}e^{-i(\phi+\lambda)/2}\cos(\theta/2) & -e^{-i(\phi-\lambda)/2}\sin(\theta/2)\\ e^{i(\phi-\lambda)/2}\sin(\theta/2) & e^{i(\phi+\lambda)/2}\cos(\theta/2)\end{pmatrix}$	$\lvert q_0\rangle$ $U3(\theta,\phi,\lambda)$
phase gate (s)	$\begin{pmatrix}1 & 0\\ 0 & i\end{pmatrix}$	$\lvert q_0\rangle$ S
phase gate† (sdag)	$\begin{pmatrix}1 & 0\\ 0 & -i\end{pmatrix}$	$\lvert q_0\rangle$ $S^\dagger$
swap gate	$\begin{pmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{pmatrix}$	$\lvert q_0\rangle$ $\lvert q_1\rangle$
CNOT gate (cx)	$\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}$	$\lvert q_0\rangle$ $\lvert q_1\rangle$
Toffoli gate (cxx)	$\begin{pmatrix}1&0&0&0&0&0&0&0\\0&1&0&0&0&0&0&0\\0&0&1&0&0&0&0&0\\0&0&0&1&0&0&0&0\\0&0&0&0&1&0&0&0\\0&0&0&0&0&1&0&0\\0&0&0&0&0&0&0&1\\0&0&0&0&0&0&1&0\end{pmatrix}$	$\lvert q_0\rangle$ $\lvert q_1\rangle$ $\lvert q_2\rangle$

Qubits, States and Complexity

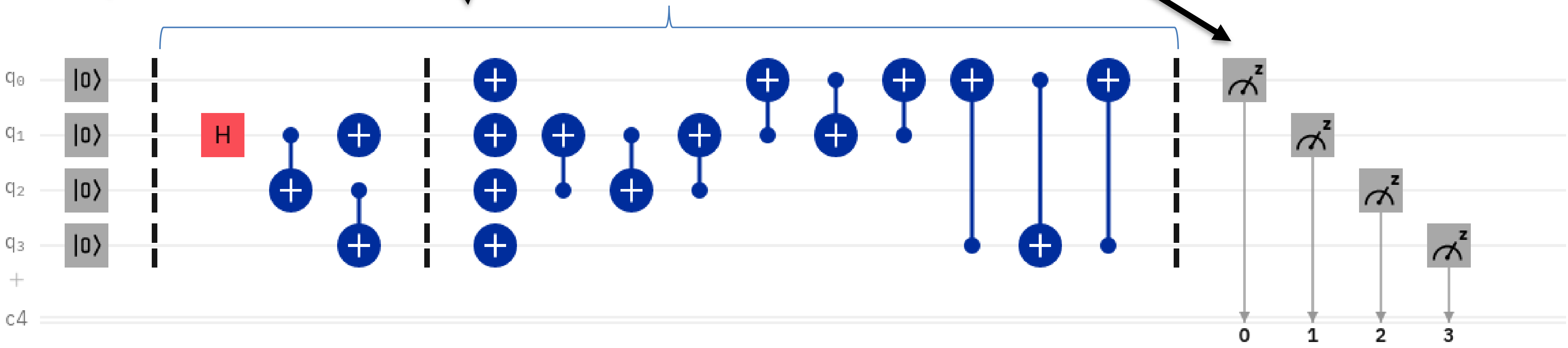
Operations on quantum states of multiple qubits: **Quantum Programs**

Build program from many small steps (quantum gates).

1. Start with a well-defined initial state, i.e., S=|00000000...⟩

2. Apply quantum gates to realise some operation.

3. Measure the probabilities.



https://quantum-computing.ibm.com/composer

Qubits, States and Complexity

Superposition for Computations:

3-qubit entangled state (GHZ-like)

$$(|0011\rangle - |0100\rangle)/\sqrt{2}$$

(7x) mod 15
modular multiplication

Resulting state is $(|0110\rangle - |1101\rangle)/\sqrt{2}$

We measure

- 0110 with 50% probability
- 1101 with 50% probability

state	x	(7x) mod 15	result
$\|0100\rangle$	4	13	$\|1101\rangle$
$\|0011\rangle$	3	6	$\|0110\rangle$

Superposition: apply one operation to many states at once!
Inherently parallel!

https://quantum-computing.ibm.com/composer

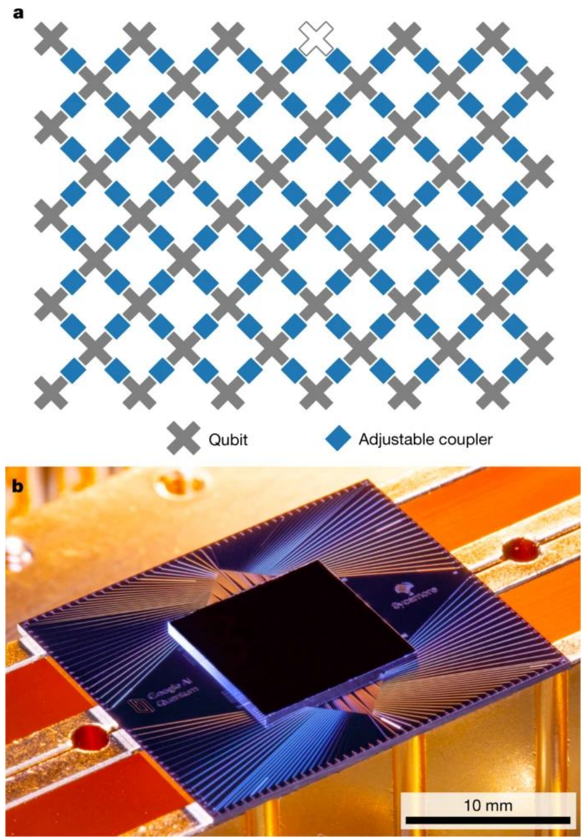
Challenges in Practice

- **Basic programming principles** and even some interesting algorithms known for several decades.

Requirements (DiVincenzo, Fortschr. Phys., 48: 771-783. 2000):

1. "a **scalable** physical system with well-characterized quantum-mechanical observables to represent the qubits,"

Sycamore quantum computer



Some physical principles of qubits:

- cooper pairs in Josephson junctions (e.g. transmon qubits)
- ions in electromagnetic traps manipulated with laser pulses,
- nuclear spins of molecules manipulated with nuclear magnetic resonance,
- single photons in non-linear optical media

Arute et al, [*Nature*] vol. 574, p. 505–510(2019)

Challenges in Practice

Requirements (DiVincenzo, Fortschr. Phys., 48: 771-783. 2000):

2. "a preparation of an **initial qubit state**,"

3. "a controllable unitary evolution with **single qubit-gates** and at least **one type of universal two-qubit gate"**

name	unitary matrix	visual representation
Hadamard gate (h)	$\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\1 & -1\end{pmatrix}$	$\lvert q_0\rangle$ — H —
σ_x gate (x)	$\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$	$\lvert q_0\rangle$ — X —
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R_y gate (ry)	$e^{-i\theta\sigma_y/2} = \begin{pmatrix}\cos(\theta/2) & -\sin(\theta/2)\\\sin(\theta/2) & \cos(\theta/2)\end{pmatrix}$	$\lvert q_0\rangle$ — $R_y(\theta)$ —
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phase shift	$e^{i\theta\mathbb{1}} = \begin{pmatrix}e^{i\theta} & 0\\0 & e^{i\theta}\end{pmatrix}$	$\lvert q_0\rangle$ — $Ph(\theta)$ —
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phase gate (s)	$\begin{pmatrix}1 & 0\\0 & i\end{pmatrix}$	$\lvert q_0\rangle$ — S —
phase gate† (sdag)	$\begin{pmatrix}1 & 0\\0 & -i\end{pmatrix}$	$\lvert q_0\rangle$ — $S^\dagger$ —
swap gate	$\begin{pmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{pmatrix}$	$\lvert q_0\rangle$ — × — $\lvert q_1\rangle$ — × —
CNOT gate (cx)	$\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}$	$\lvert q_0\rangle$ — ● — $\lvert q_1\rangle$ — ⊕ —
Toffoli gate (cxx)	$\begin{pmatrix}1&0&0&0&0&0&0&0\\0&1&0&0&0&0&0&0\\0&0&1&0&0&0&0&0\\0&0&0&1&0&0&0&0\\0&0&0&0&1&0&0&0\\0&0&0&0&0&1&0&0\\0&0&0&0&0&0&0&1\\0&0&0&0&0&0&1&0\end{pmatrix}$	$\lvert q_0\rangle$ — ● — $\lvert q_1\rangle$ — ● — $\lvert q_2\rangle$ — ⊕ —

Challenges in Practice

Requirements (DiVincenzo, Fortschr. Phys., 48: 771-783. 2000):

4. "**decoherence times** that are much longer than gate-operation times"

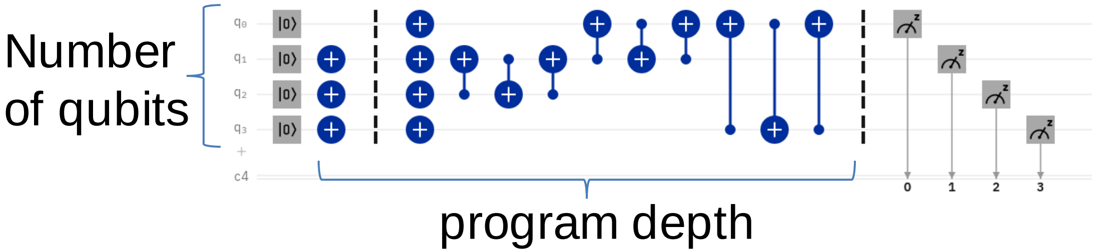
Decoherence time: The duration for which the quantum state can keep its **quantum nature**.
So basically the **time available to compute**.

- Noise from finite temperature
- Noise from external electric and magnetic fields
- Crosstalk between qubits
- …..

Challenges in Practice

Requirements (DiVincenzo, Fortschr. Phys., 48: 771-783. 2000):

4. **decoherence times** that are much longer than gate-operation times



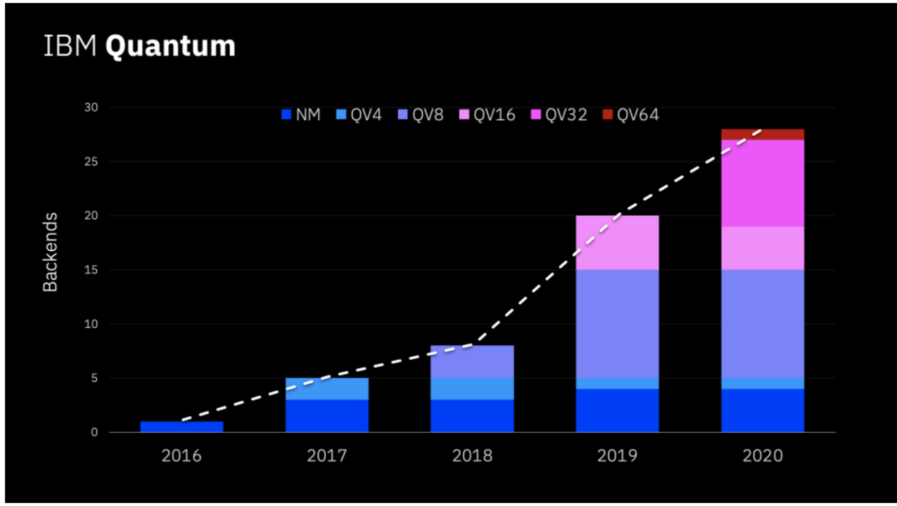
$$V \geq 4 \cdot 11 = 44$$

Power of a QC can be quantified with the **quantum volume V** (Moll, 2017):

- Number of qubits, decoherence times
- gate- and measurement error rates
- Connectivity of qubits

Example (with a grain of salt):

A value of V means that it can run any program where the product of **program depth and number of qubits** is smaller than V.



Source: IBM

An Interesting Algorithm for an HPC Workload

- Initially, most quantum algorithms assumed **perfect quantum computers.**
- Then **quantum error correction** schemes have been developed

  But **many qubits** needed and **long programs**.

New idea in the last ten years:

Simulate a quantum system (e.g. molecules) on quantum computers in a noise-tolerant way.

An Interesting Algorithm for an HPC Workload

<u>Quantum computer</u>

New idea in the last ten years:

Simulate a quantum system (e.g. molecules) on quantum computers in a noise-tolerant way.

Variational Classical Eigensolvers

(VASP, CP2K, Gaussian,…)

$$E_{GS} = \min_{\vec{x}} E(\Psi(\vec{x}))$$

i.e. minimize the energy to find the ground state.

* Note: depending on the level of theory (DFT, CCSD(T),…) the wave functions are single-particle wave functions or many-particle wave functions.

An Interesting Algorithm for an HPC Workload

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Quantum computer

Variational Quantum Eigensolver (VQE)

(VQE, Peruzzo et. al, 2013)

$$E_{GS} = \min_{\vec{x}} E(\Psi(\vec{x}))$$

i.e. minimize the energy to find the ground state.
Parameters are optimized on the classical computer.

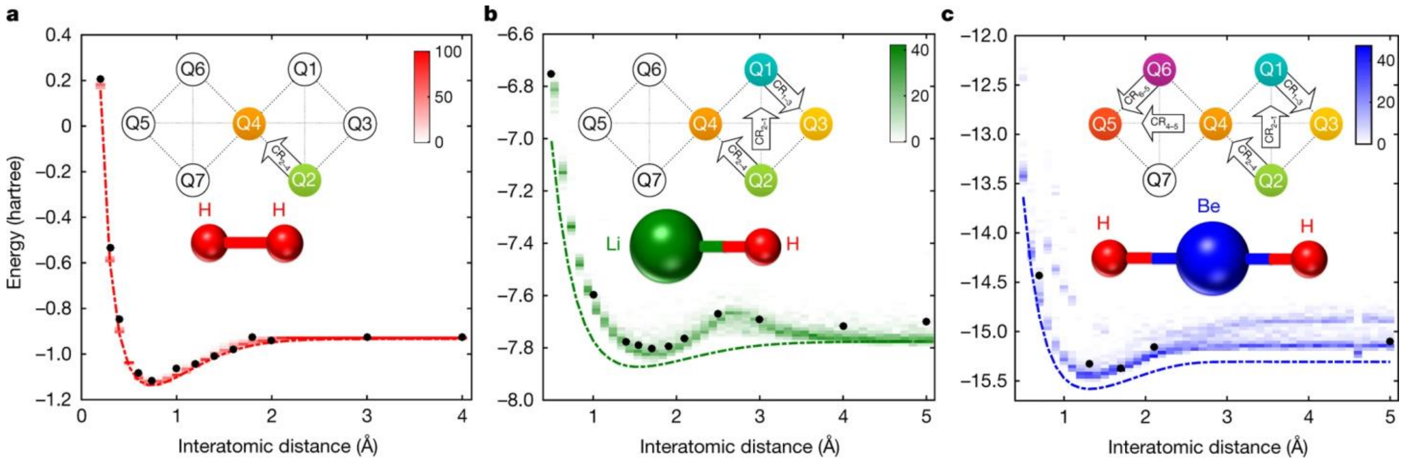
BUT: Energy is calculated on the QC!

- automatically compensates crosstalk and shifts
- **noise-tolerant***
- Even 35-100 qubits can give results that no supercomputer can.

* Note: depending on the level of theory (DFT, CCSD(T),…) the wave functions are single-particle wave functions or many-particle wave functions.

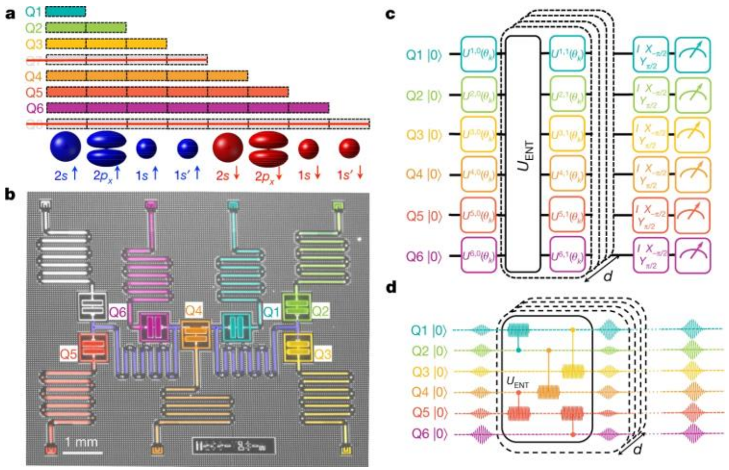
An Interesting Algorithm for an HPC Workload

Variational Quantum Eigensolver (VQE, Peruzzo et. al, 2013):



Kandala et. al, [*Nature*]() **vol. 549**, p. 242–246 (2017)

$$E_{GS} = \min_{\vec{x}} E(\Psi(\vec{x}))$$



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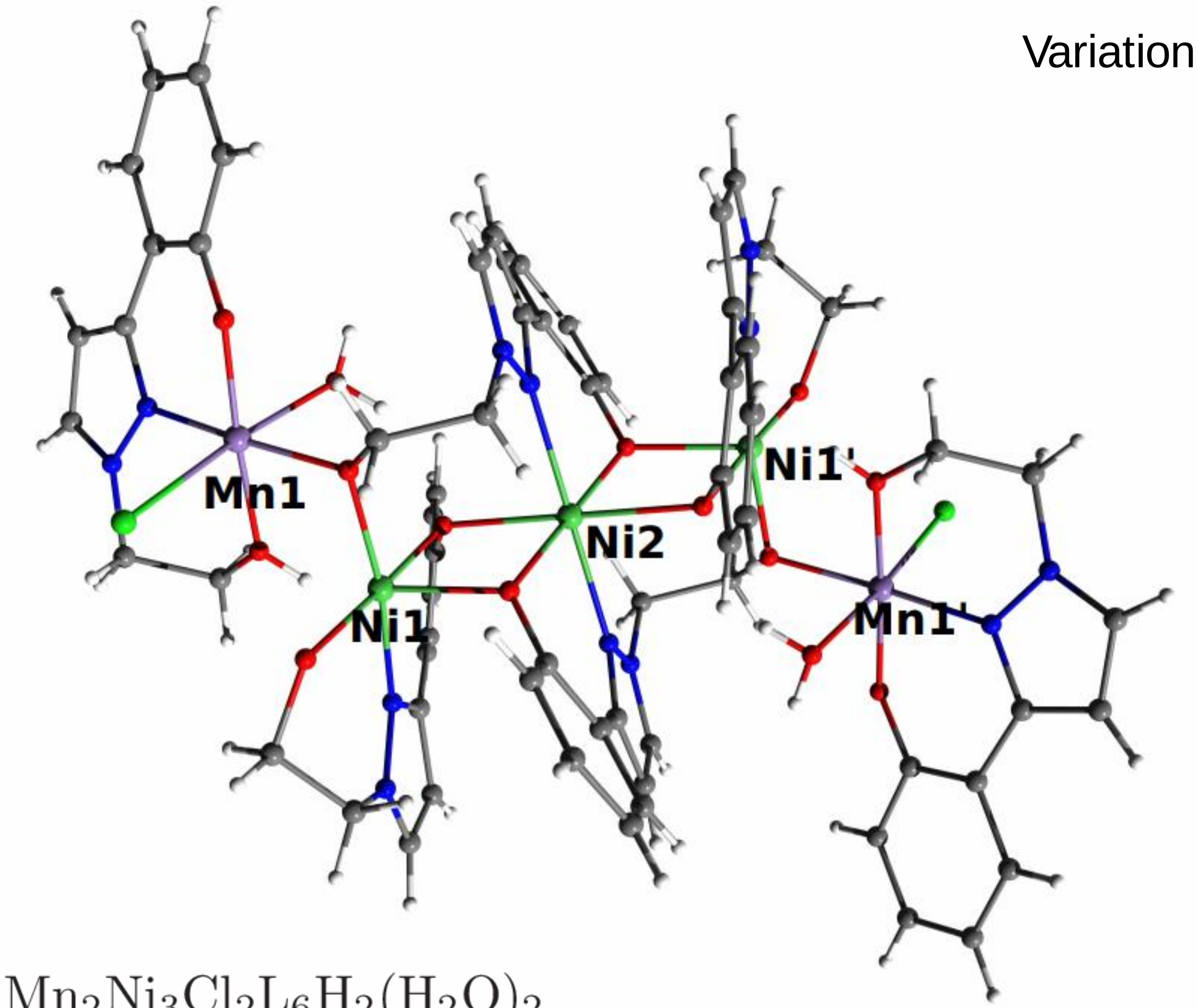
An Interesting Algorithm for an HPC Workload

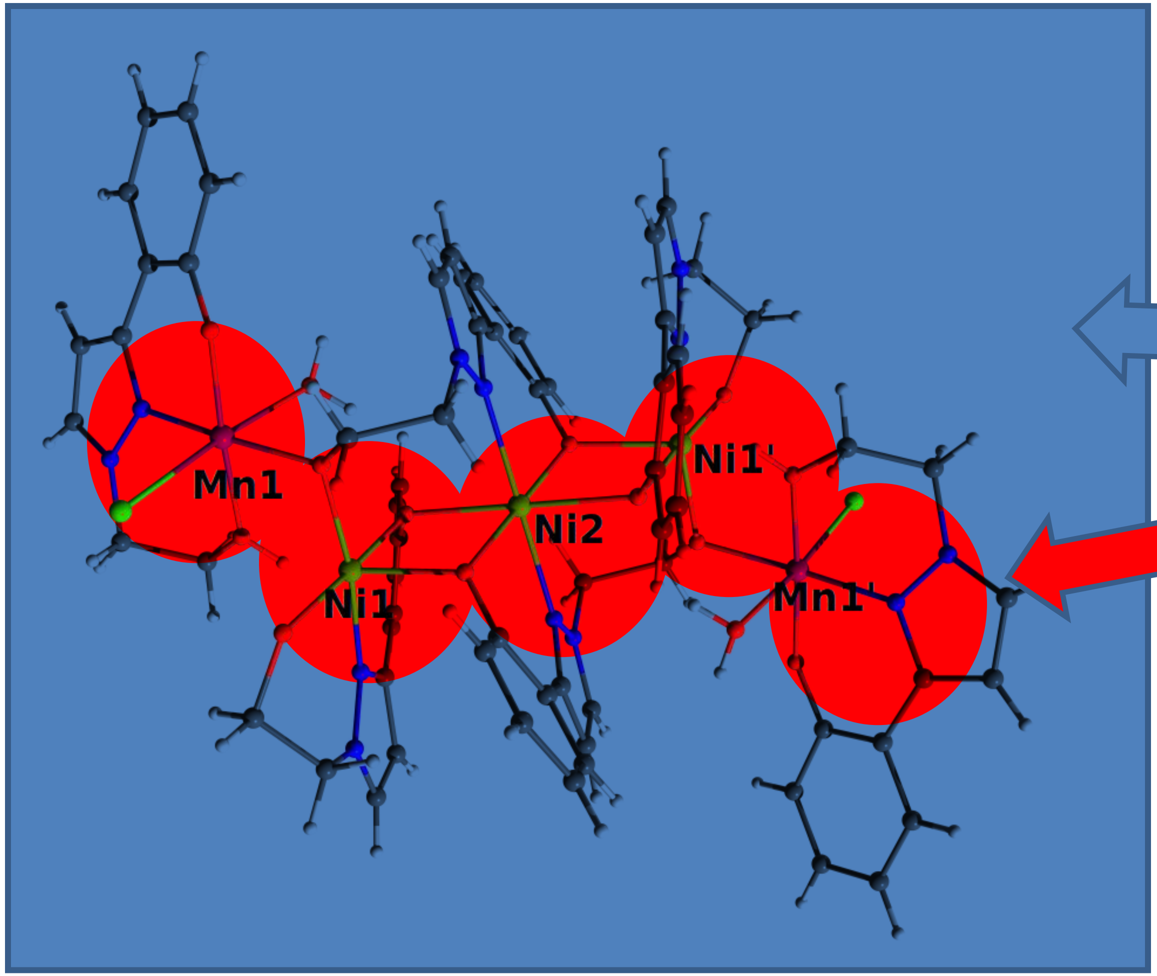
Variational Quantum Eigensolver: ~500 qubits required



$Mn_2Ni_3Cl_2L_6H_2(H_2O)_2$

Das et al., *J. Am. Chem. Soc.* 2011, 133, 10, 3433–3443

An Interesting Algorithm for an HPC Workload



Variational Quantum Eigensolver: ~500 qubits required

Idea: decompose the molecule

Outer part: Treated with approx. DFT methods on a classical computer (cubic or linear scaling)

Inner part: Treated with VQE-like algorithm on QC requires only ~90 qubits

Decomposition can be performed consistently based on the reduced density-matrix functional

Decomposition: Schade et al, EPJ ST **226**, 2677 (2017)
Solution of inner part on QC: Schade et al. in preparation, initial results in 10.5281/zenodo.4022026

$\mathrm{Mn_2Ni_3Cl_2L_6H_2(H_2O)_2}$

Das et al., *J. Am. Chem. Soc.* 2011, 133, 10, 3433–3443

Outlook

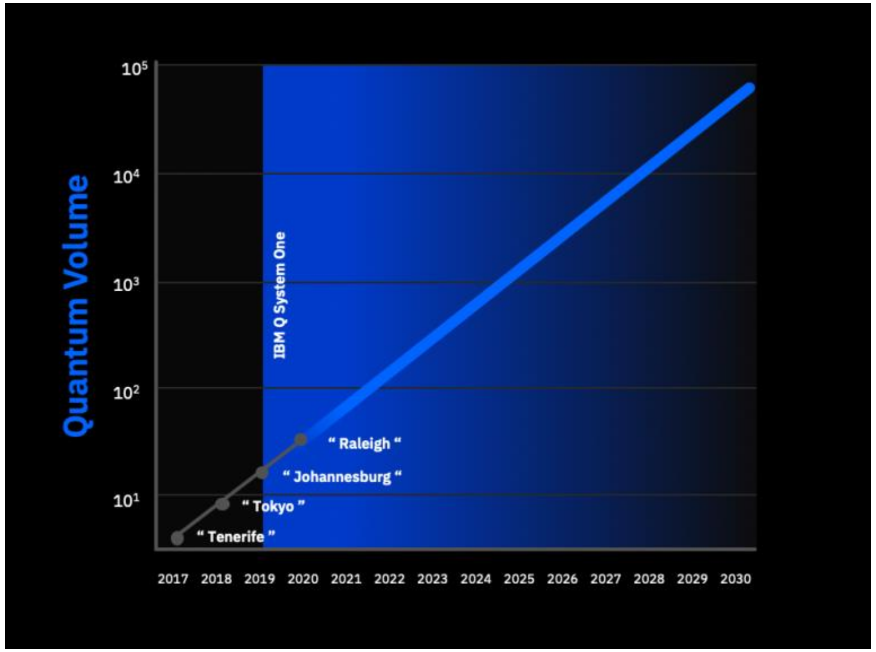
- Hopefully an **exponential increase** in quantum volume.
- An interesting race to increase quantum volume. (Many big players: IBM, Google, Microsoft, Rigetti, …

- Thankfully, **post-quantum cryptography** is already well developed.
- Quantum supremacy for useful workloads is only a matter of time.

- Creativity: Many new clever algorithms expected.

- **Chemistry / Physics / Biology**:
  - Most of the algorithmic developments of the last 90 years have to be thrown away.
  - But many new oportunities for hybrid-quantum-classical algorithms.
  - Probably some real HPC workloads run on QCs by 2030.

- Unfortunately a lot of buzzword-bingo to come: "Quantum AI"



Source: https://www.ibm.com/blogs/research/2020/01/quantum-volume-32/