Center for Quantum Devices

Kvantecomputer udvikling
En opdatering fra frontlinjerne

Morten Kjaergaard
Niels Bohr Instituttet

DIREC — IDA — ATV
06/05/2022

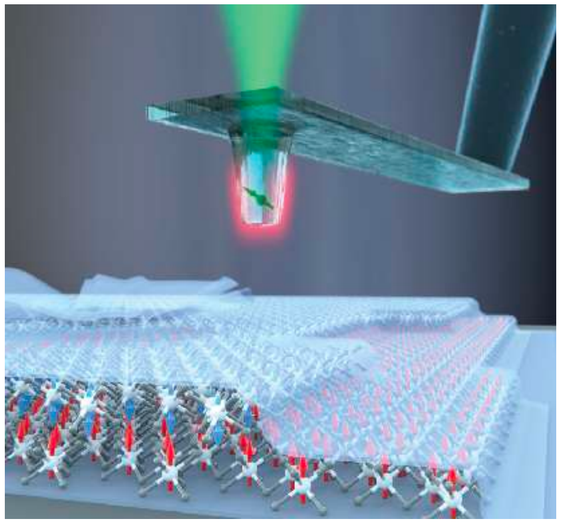
Danmarks Grundforskningsfond
Danish National Research Foundation

VILLUM FONDEN

CARLSBERGFONDET

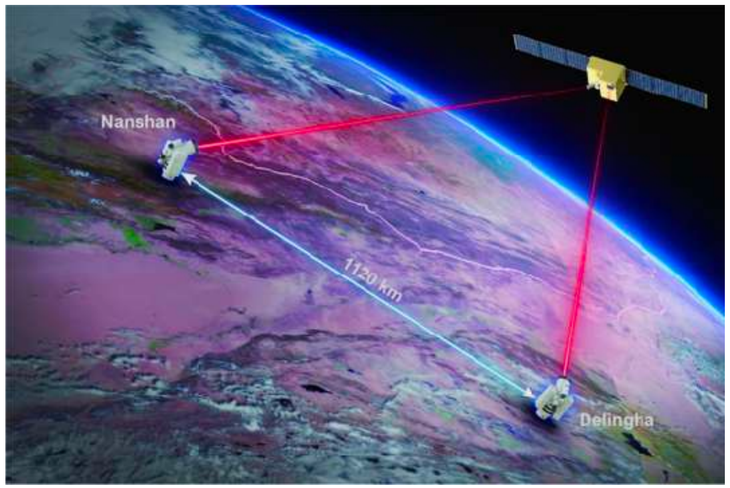
SCIENCE TO SHAPE THE FUTURE OF THE ARMY
ARMY RESEARCH OFFICE
1951

Next-generation teknologi der udnytter kvantefysikkens love



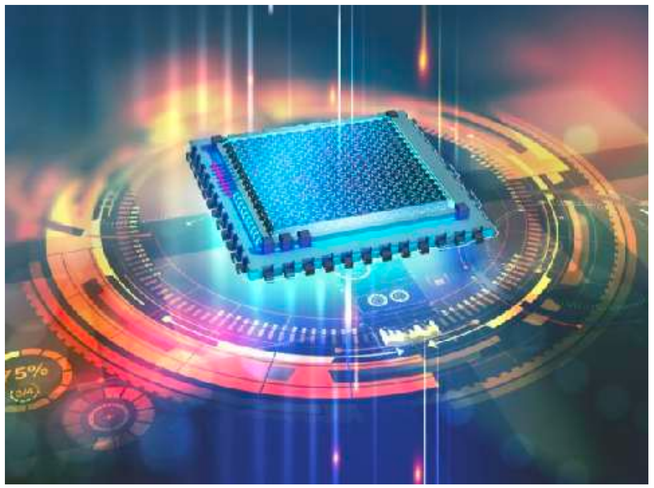
Kvantesensing

Ekstremt præcist måle-apparatur



Kvantekommunikation

Ubrydelig kommunikation



Kvantecomputere

Lynhurtige beregninger

Kvantecomputer applikation fra energi sektoren

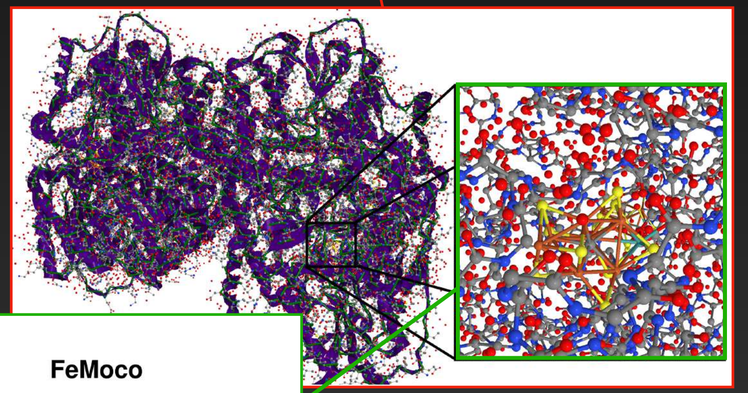
Haber-Bosch process

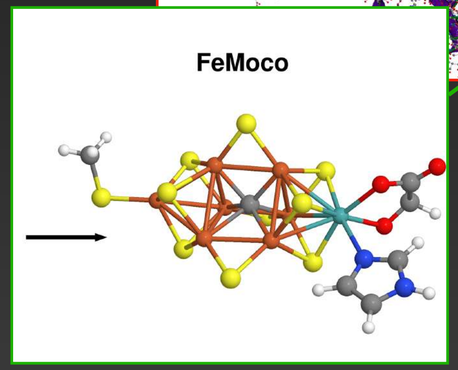
$$N_2 + 3H_2 \longrightarrow 2NH_3$$

~500C og ~300 Bar

Cirka *1% af jordens samlede energi forbrug går til HB process (!)*

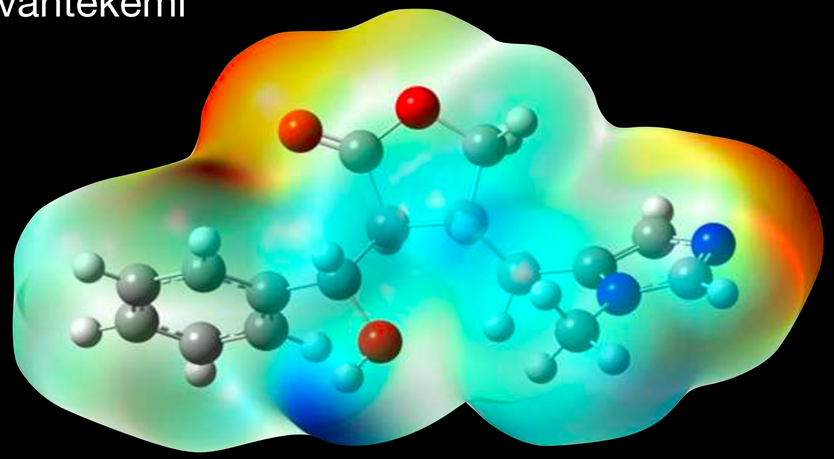
Rhizobia bakterie





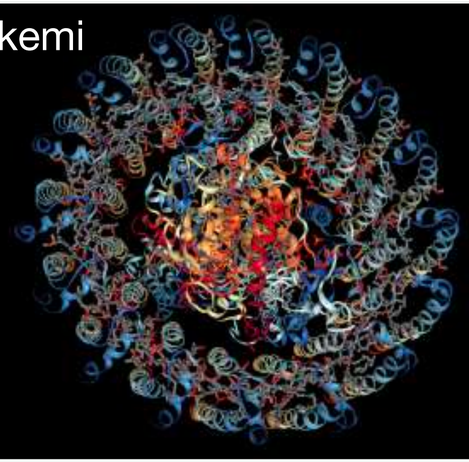
Mere generelt: Hvor forventer vi kvantecomputer ‘speedup’

Kvantekemi



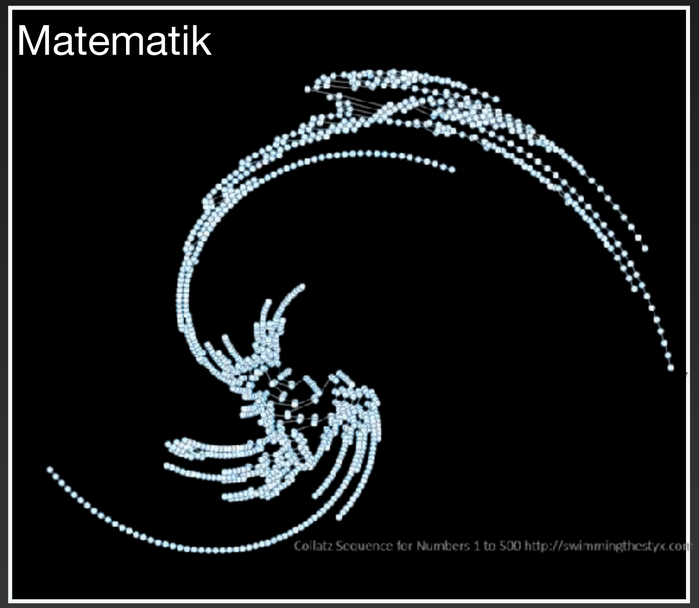
Relevant for kemisk industri/grøn omstilling

Biokemi



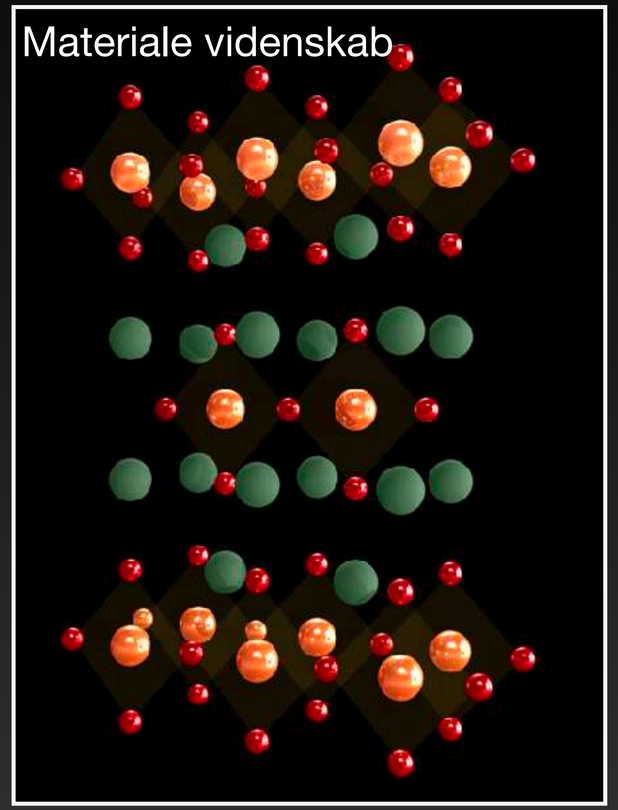
Relevant for life science sektor

Matematik



Relevant for data science/machine learning

Materiale videnskab



Relevant for grøn omstilling

Computere med (kvante) bits

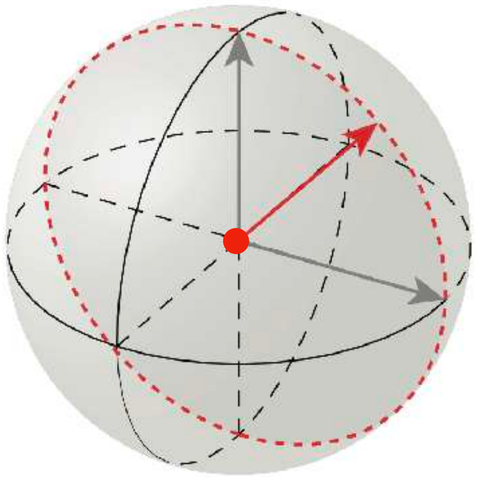
En klassisk bit

1 (‘tændt’)

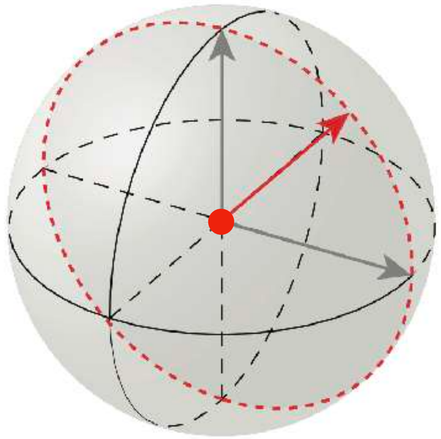
0 (‘slukket’)

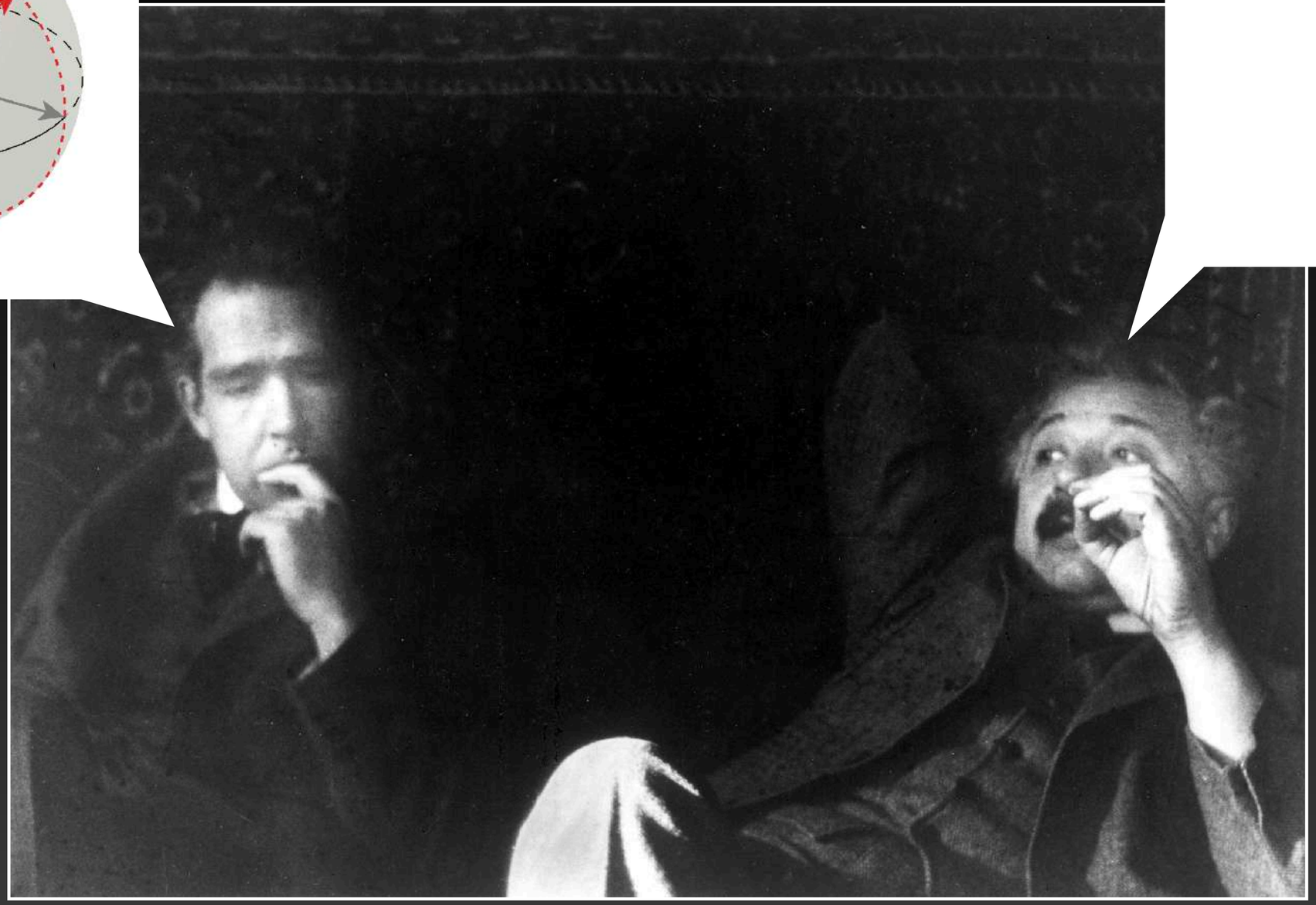
En kvantebit

$|1\rangle$



$|0\rangle$

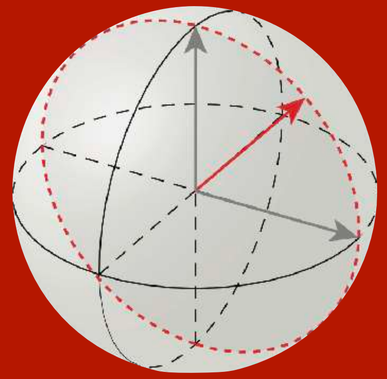




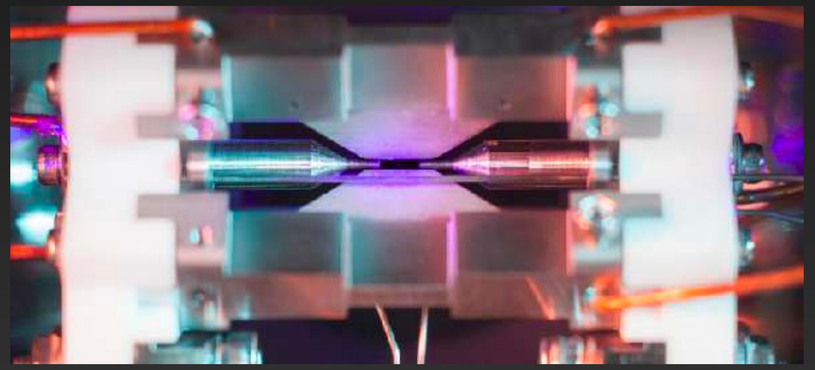
Niels Bohr

Albert Einstein

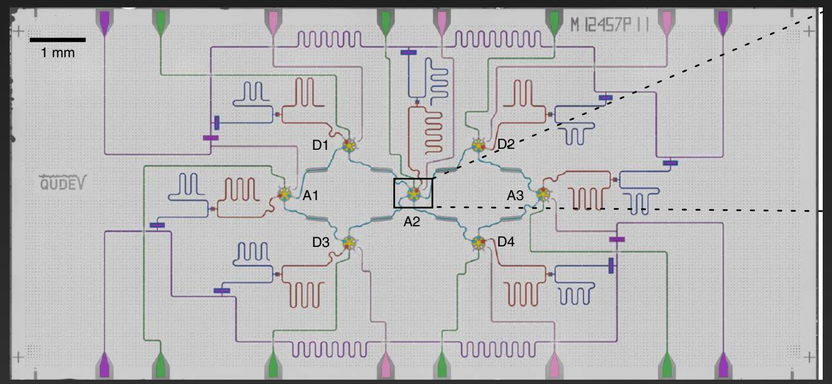
Krav til kvantebits



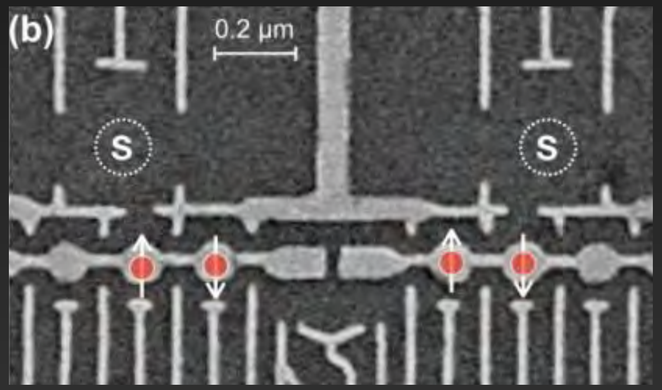
1: Fastholde ‘superposition’
2: Være kontrollerbare



Fangede ioner



Superledende kvantekredsløb

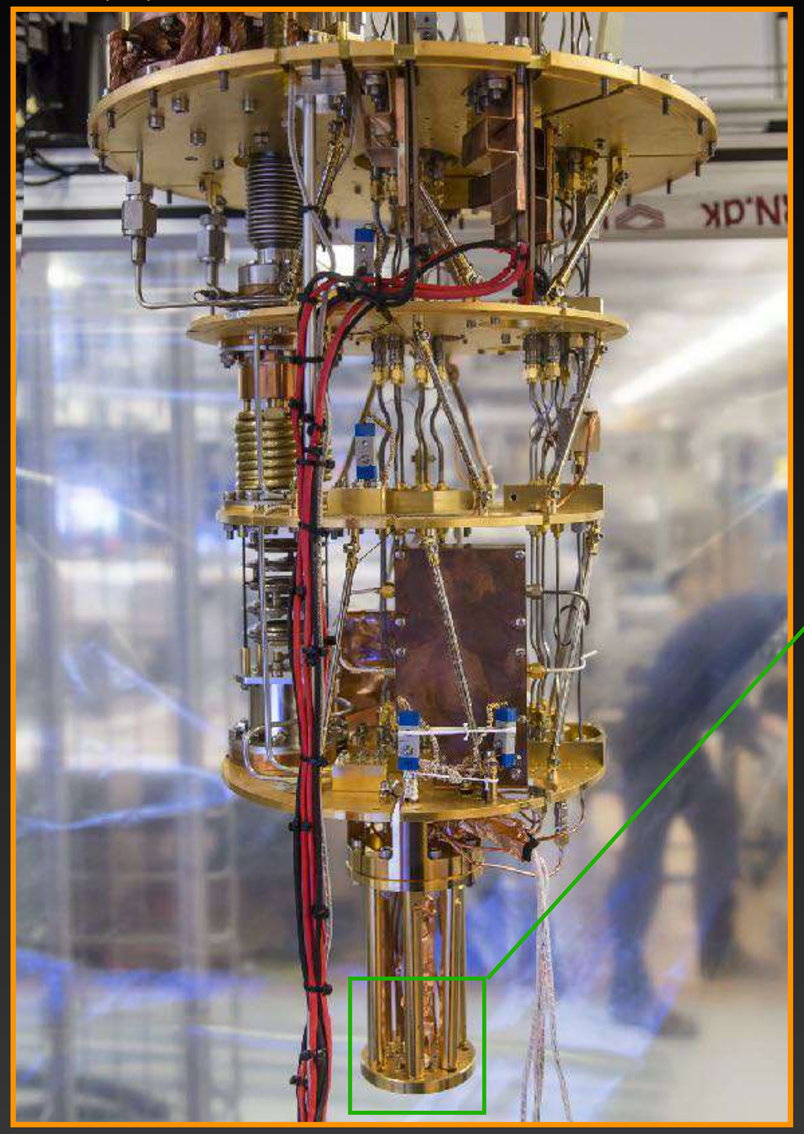


Isolerede elektroner

... mange andre

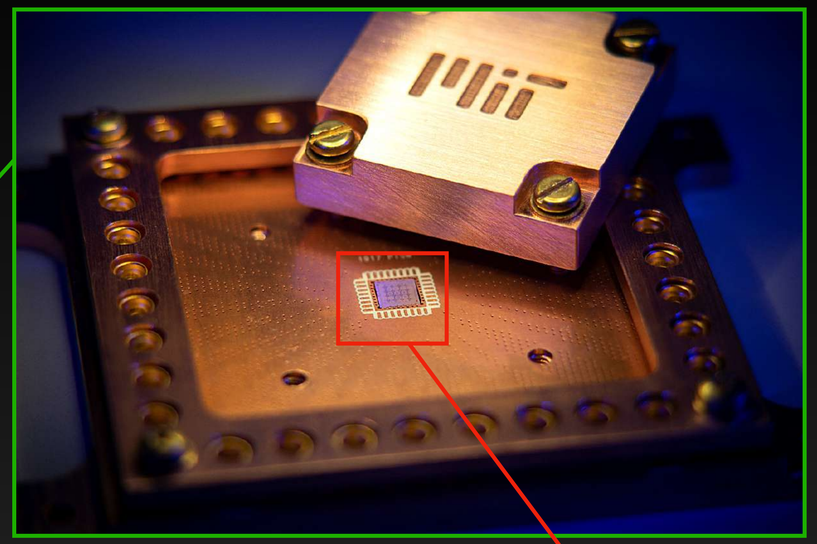
Hvordan ser en (superledende) kvantecomputer ud?

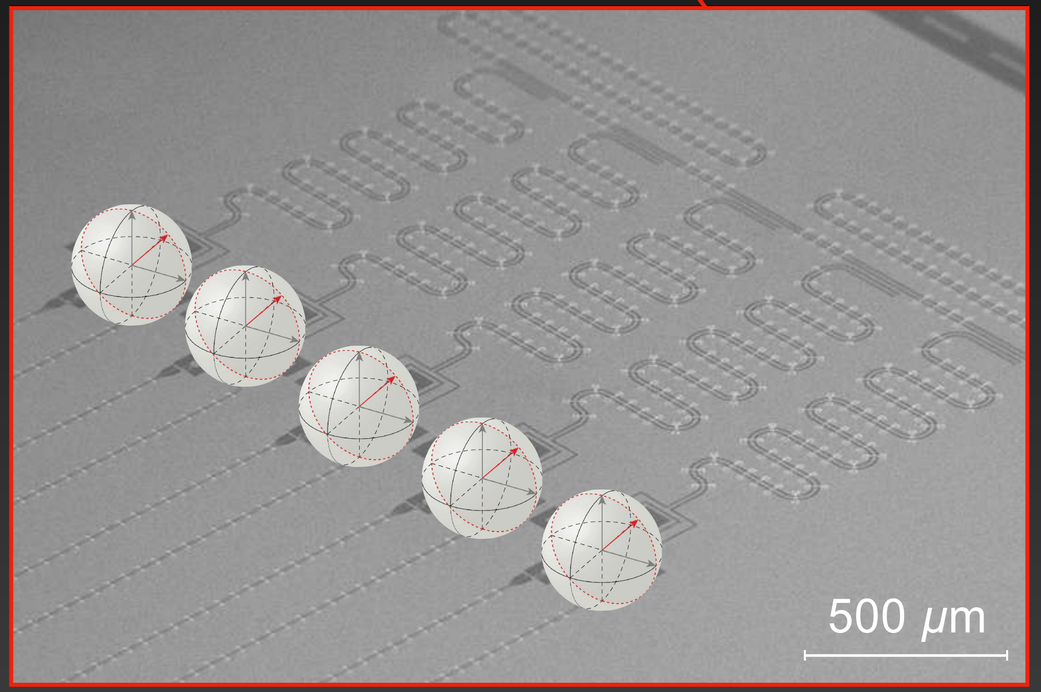
QDev (KU)



-273.1C

EQuS (MIT)





Et eksempel fra frontlinjerne

Article | Published: 23 October 2019

Quantum supremacy using a programmable superconducting processor

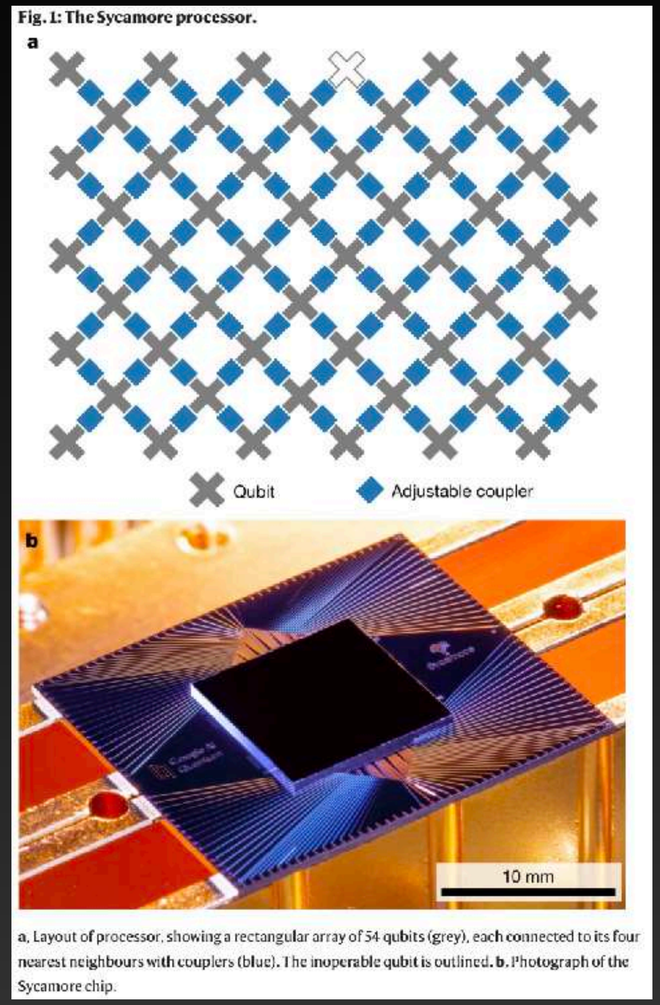
Frank Arute, Kunal Arya, [...] John M. Martinis

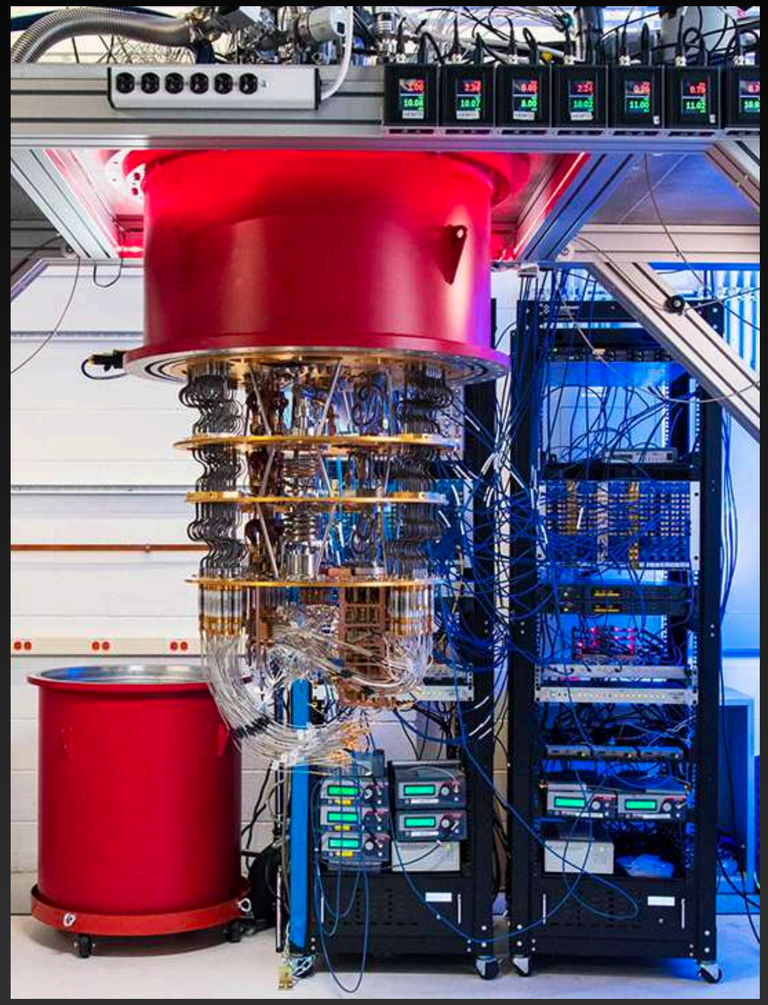
Nature **574**, 505–510 (2019) | Cite this article

870k Accesses | **1393** Citations | **6145** Altmetric | Metrics

Abstract

The promise of quantum computers is that certain computational tasks might be executed exponentially faster on a quantum processor than on a classical processor[1]. A fundamental challenge is to build a high-fidelity processor capable of running quantum algorithms in an exponentially large computational space. Here we report the use of a processor with programmable superconducting qubits[2,3,4,5,6,7] to create quantum states on 53 qubits, corresponding to a computational state-space of dimension 2^{53} (about 10^{16}). Measurements from repeated experiments sample the resulting probability distribution, which we verify using classical simulations. Our Sycamore processor takes about 200 seconds to sample one instance of a quantum circuit a million times—our benchmarks currently indicate that the equivalent task for a state-of-the-art classical supercomputer would take approximately 10,000 years. This dramatic increase in speed compared to all known classical algorithms is an experimental realization of quantum supremacy[8,9,10,11,12,13,14] for this specific computational task, heralding a much-anticipated computing paradigm.





Google Quantum AI

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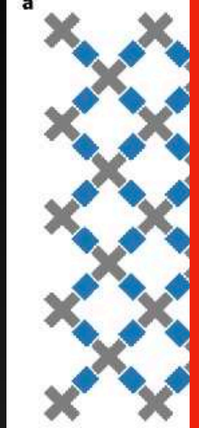
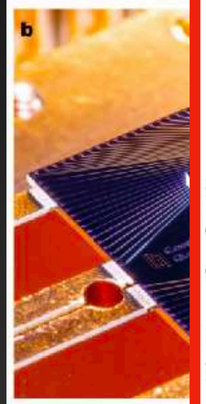
Fig. 1: The Sycamore pr





a, Layout of processor, sho
nearest neighbours with co
Sycamore chip.

Google Quar

Quantum Computing

On "Quantum Supremacy"

October 21, 2019 | Written by: Edwin Pednault, John Gunnels & Dmitri Maslov, and Jay Gambetta

Categorized: Quantum Computing

Quantum computers are starting to approach the limit of classical simulation and it is important that we continue to benchmark progress and to ask how difficult they are to simulate. This is a fascinating scientific question.

Recent advances in quantum computing have resulted in two 53-qubit processors: one from our group in IBM and a device described by Google in a paper published in the journal *Nature*. In the paper, it is argued that their device reached "quantum supremacy" and that "a state-of-the-art supercomputer would require approximately 10,000 years to perform the equivalent task." *We argue that an ideal simulation of the same task can be performed on a classical system in 2.5 days and with far greater fidelity.* This is in fact a conservative, worst-case estimate, and we expect that with additional refinements the classical cost of the simulation can be further reduced.

IBM Quantum

Kinesisk bud på quantum supremacy

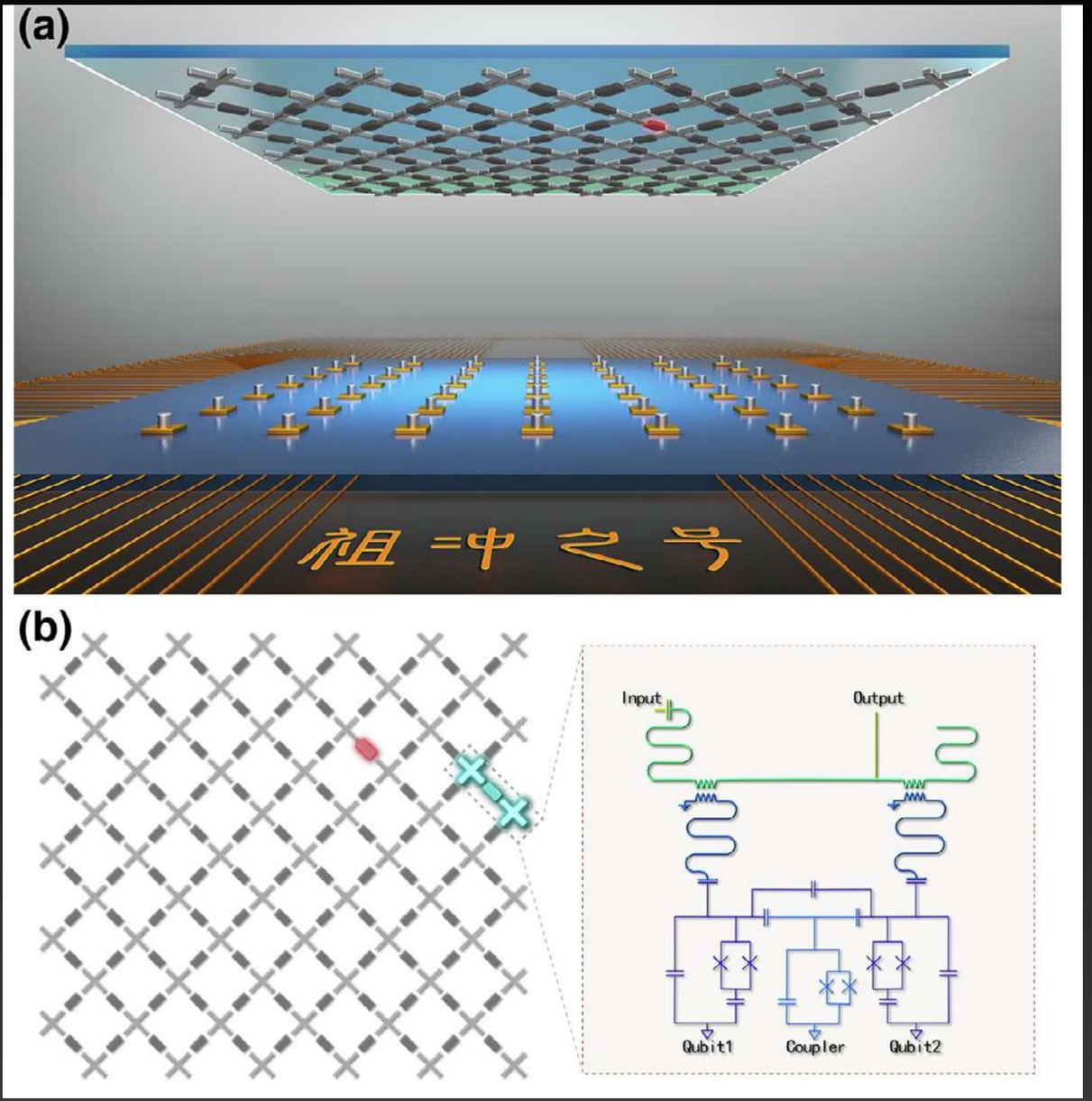
Quantum Computational Advantage via 60-Qubit 24-Cycle Random Circuit Sampling

Qingling Zhu,[1,2,3] Sirui Cao,[1,2,3] Fusheng Chen,[1,2,3] Ming-Cheng Chen,[1,2,3] Xiawei Chen,[2] Tung-Hsun Chung,[1,2,3] Hui Deng,[1,2,3] Yajie Du,[2] Daojin Fan,[1,2,3] Ming Gong,[1,2,3] Cheng Guo,[1,2,3] Chu Guo,[1,2,3] Shaojun Guo,[1,2,3] Lianchen Han,[1,2,3] Linyin Hong,[4] He-Liang Huang,[1,2,3,5] Yong-Heng Huo,[1,2,3] Liping Li,[2] Na Li,[1,2,3] Shaowei Li,[1,2,3] Yuan Li,[1,2,3] Futian Liang,[1,2,3] Chun Lin,[6] Jin Lin,[1,2,3] Haoran Qian,[1,2,3] Dan Qiao,[2] Hao Rong,[1,2,3] Hong Su,[1,2,3] Lihua Sun,[1,2,3] Liangyuan Wang,[2] Shiyu Wang,[1,2,3] Dachao Wu,[1,2,3] Yulin Wu,[1,2,3] Yu Xu,[1,2,3] Kai Yan,[2] Weifeng Yang,[4] Yang Yang,[2] Yangsen Ye,[1,2,3] Jianghan Yin,[2] Chong Ying,[1,2,3] Jiale Yu,[1,2,3] Chen Zha,[1,2,3] Cha Zhang,[1,2,3] Haibin Zhang,[2] Kaili Zhang,[1,2,3] Yiming Zhang,[1,2,3] Han Zhao,[2] Youwei Zhao,[1,2,3] Liang Zhou,[4] Chao-Yang Lu,[1,2,3] Cheng-Zhi Peng,[1,2,3] Xiaobo Zhu,[1,2,3] and Jian-Wei Pan[1,2,3]

[1]*Hefei National Laboratory for Physical Sciences at the Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei 230026, China*
[2]*Shanghai Branch, CAS Center for Excellence in Quantum Information and Quantum Physics, University of Science and Technology of China, Shanghai 201315, China*
[3]*Shanghai Research Center for Quantum Sciences, Shanghai 201315, China*
[4]*QuantumCTek Co., Ltd., Hefei 230026, China*
[5]*Henan Key Laboratory of Quantum Information and Cryptography, Zhengzhou 450000, China*
[6]*Shanghai Institute of Technical Physics, Chinese Academy of Sciences, Shanghai 200083, China*

9 Sept 2021

To ensure a long-term quantum computational advantage, the quantum hardware should be upgraded to withstand the competition of continuously improved classical algorithms and hardwares. Here, we demonstrate a superconducting quantum computing systems *Zuchongzhi* 2.1, which has 66 qubits in a two-dimensional array in a tunable coupler architecture. The readout fidelity of *Zuchongzhi* 2.1 is considerably improved to an average of 97.74%. The more powerful quantum processor enables us to achieve larger-scale random quantum circuit sampling, with a system scale of up to 60 qubits and 24 cycles. The achieved sampling task is about 6 orders of magnitude more difficult than that of Sycamore [Nature **574**, 505 (2019)] in the classic simulation, and 3 orders of magnitude more difficult than the sampling task on *Zuchongzhi* 2.0 [arXiv:2106.14734 (2021)]. The time consumption of classically simulating random circuit sampling experiment using state-of-the-art classical algorithm and supercomputer is extended to tens of thousands of years (about 4.8×10^4 years), while *Zuchongzhi* 2.1 only takes about 4.2 hours, thereby significantly enhancing the quantum computational advantage.



Kommercielle interesser har drevet kvantecomputer *skalering*

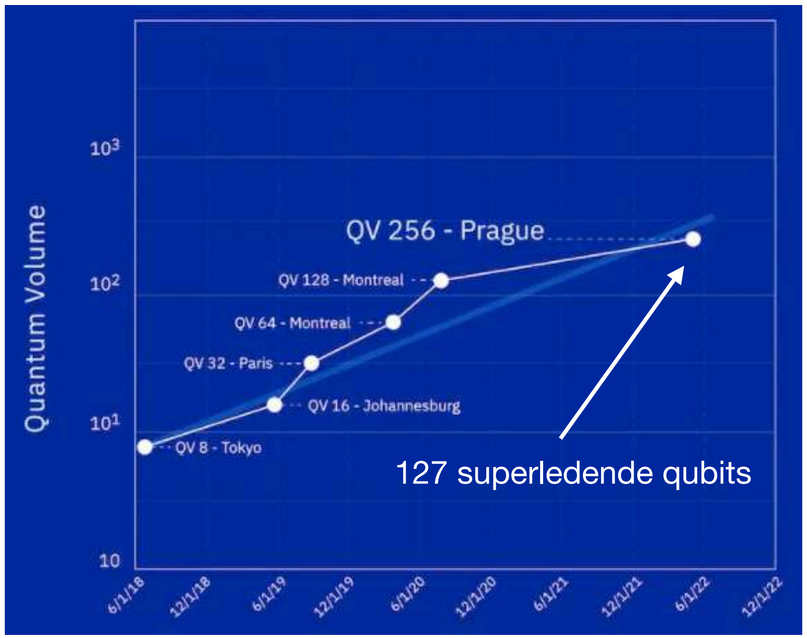
News 5 minute read

Date
06 Apr 2022

Pushing quantum performance forward with our highest Quantum Volume yet

Authors
Petar Jurcevic
David Zajac
Jiri Stehlik
Isaac Lauer
Ryan Mandelbaum

IBM Quantum has once again doubled the Quantum Volume of our highest-performing processor, achieving a Quantum Volume of 256 on the Falcon r10.



IBM Press release fra starten af april

ABOUT DEVELOPERS PRODUCTS RESEARCHERS CAREERS PARTNERS

Demonstrating Benefits of Quantum Upgradable Design Strategy: System Model H1-2 First to Prove 2,048 Quantum Volume

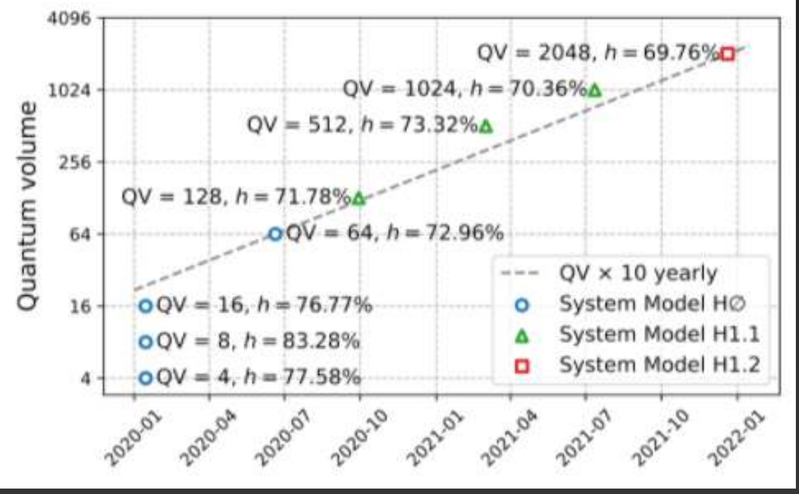
December 29, 2021

Contact:

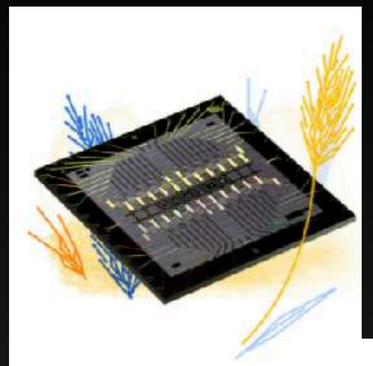
Media
Kortny Rolston-Duce
+1 (208) 522-4809
Kortny.rolston-duce@honeywell.com

Demonstrating Benefits of Quantum Upgradable Design Strategy: System Model H1-2 First to Prove 2,048 Quantum Volume

Quantinuum's H-Series quantum computers, Powered by Honeywell, continue to deliver on exponential performance gains

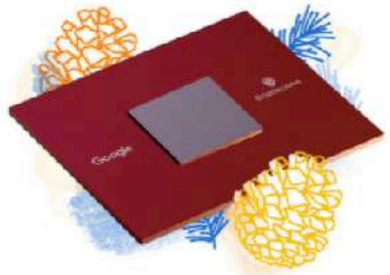


Honeywell (Quantinuum)



Foxtail (2016)

22 qubits



Bristlecone (2017)

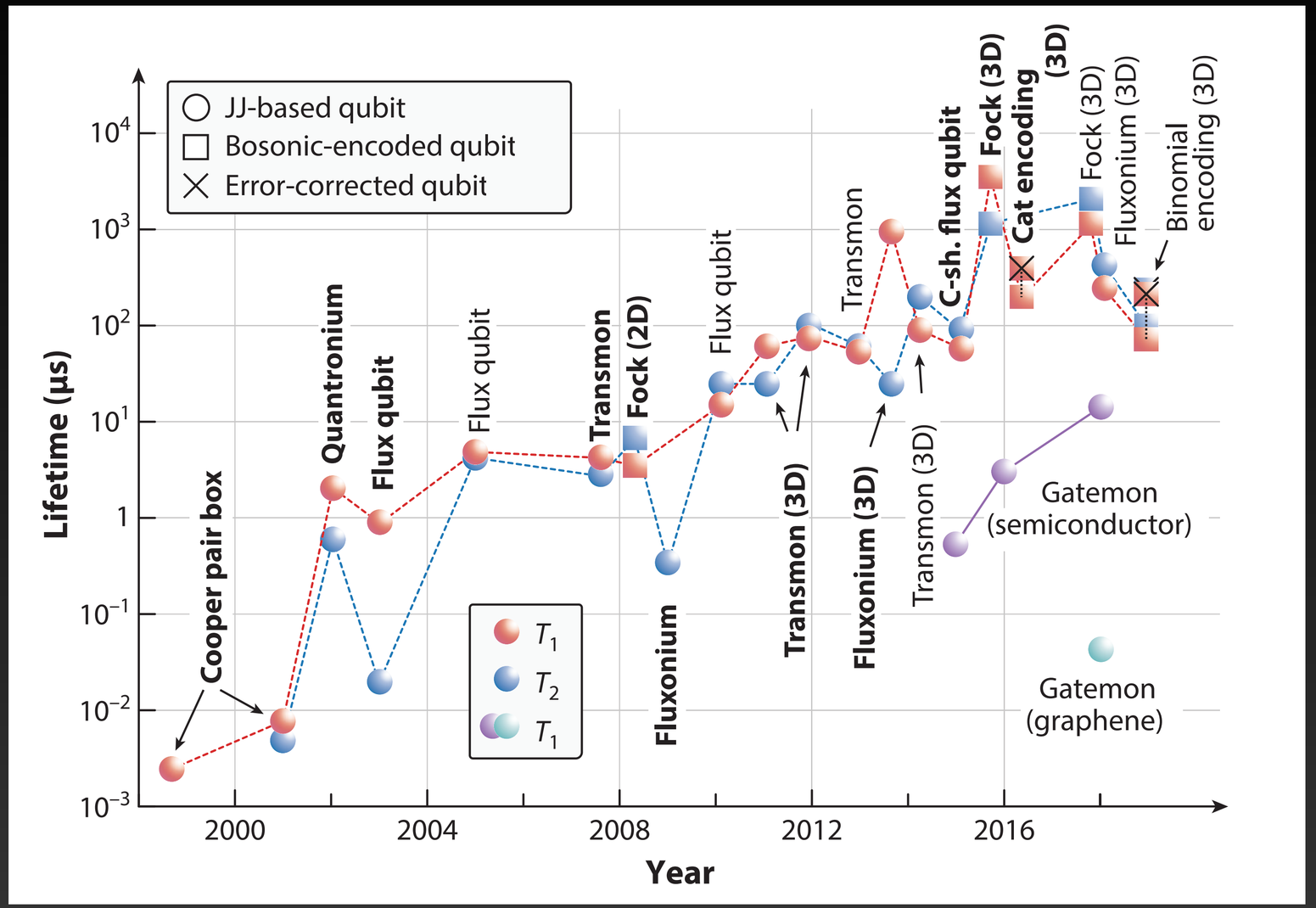
72 qubits

Sycamore (2018)

53 qubits (better control)

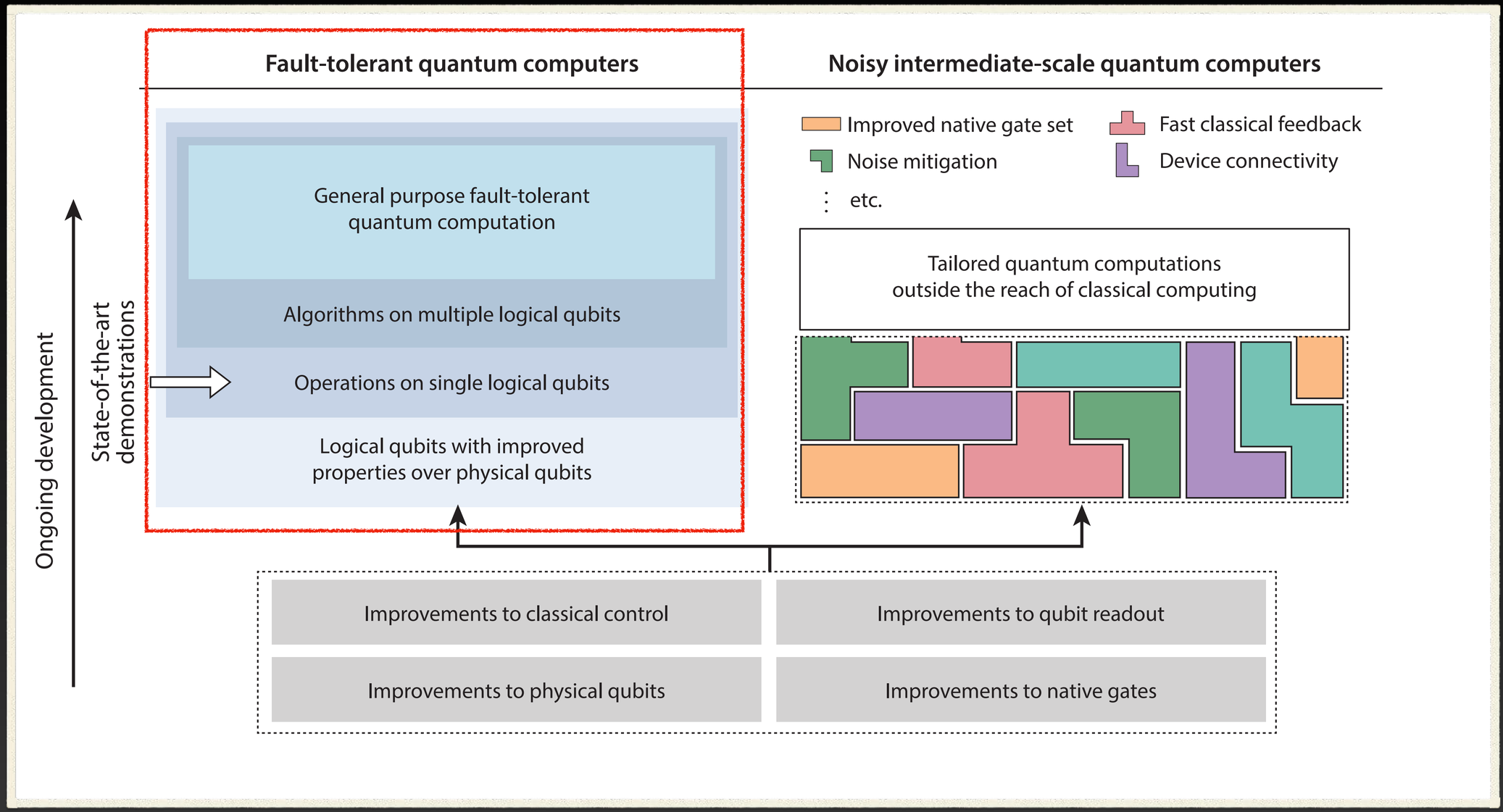
Google Quantum AI

Fundamental kvantehardwareudvikling anført af akademisk forskning



Fra Kjaergaard et al, Ann. Rev. Cond. Matt. (2022)

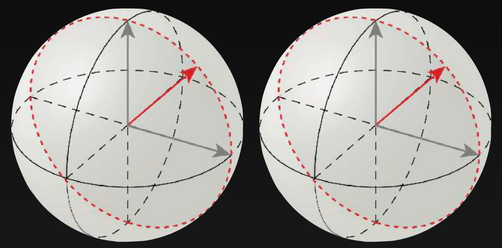
Den fremtidige udvikling af kvantecomputere



Fra Kjaergaard et al, Ann. Rev. Cond. Matt. (2022)

Hvor bliver den store kvantecomputer af?

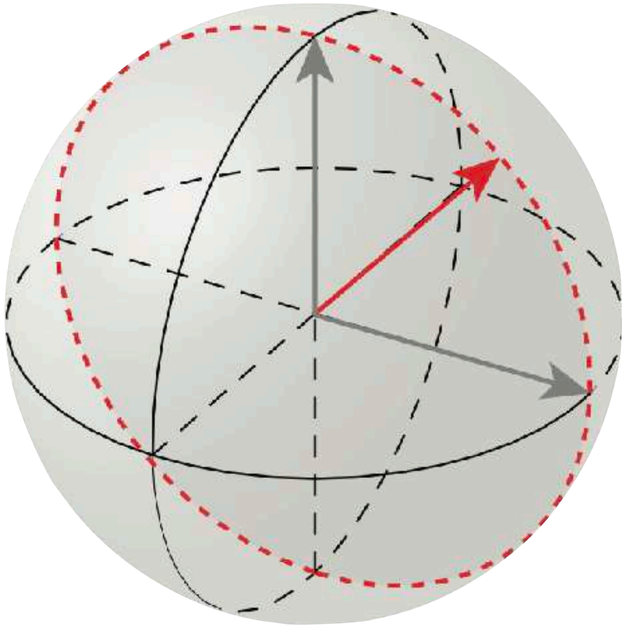
Qubits er meget meget følsomme overfor støj



Fejlretning bliver en absolut nødvendighed

Redundans nedsætter følsomhed til støj

Med fejlrate på cirka 0.1%: 2000 *fysiske* (fejlfyldte) qubits



1 *logisk* (fejlfri) qubit

From Lee et al, PRX Quantum, (2021)

Hvor langt er vi med fejlretning?

nature physics

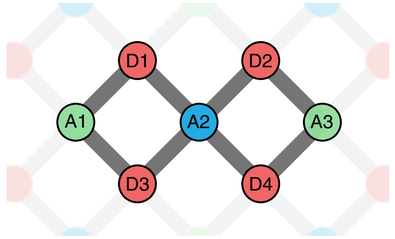
ARTICLES

https://doi.org/10.1038/s41567-020-0920-y

Check for updates

Repeated quantum error detection in a surface code

Christian Kraglund Andersen ✉, Ants Remm, Stefania Lazar, Sebastian Krinner, Nathan Lacroix, Graham J. Norris, Mihai Gabureac, Christopher Eichler and Andreas Wallraff



August 2020

Logical-qubit operations in an error-detecting surface code

J. F. Marques,[1,2] B. M. Varbanov,[1] M. S. Moreira,[1,2] H. Ali,[1,2] N. Muthusubramanian,[1,2] C. Zachariadis,[1,2] F. Battistel,[1] M. Beekman,[1,3] N. Haider,[1,3] W. Vlothuizen,[1,3] A. Bruno,[1,2] B. M. Terhal,[1,4] and L. DiCarlo[1,2]

[1] *QuTech, Delft University of Technology, P.O. Box 5046, 2600 GA Delft, The Netherlands*
[2] *Kavli Institute of Nanoscience, Delft University of Technology, P.O. Box 5046, 2600 GA Delft, The Netherlands*
[3] *Netherlands Organisation for Applied Scientific Research (TNO), P.O. Box 96864, 2509 JG The Hague, The Netherlands*
[4] *JARA Institute for Quantum Information, Forschungszentrum Juelich, D-52425 Juelich, Germany*

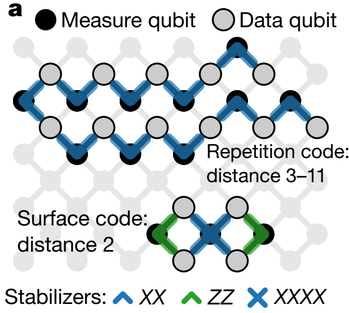
(Dated: February 26, 2021)

February 2021

Article

Exponential suppression of bit or phase errors with cyclic error correction

Google Quantum AI*



July 2021

Realization of an Error-Correcting Surface Code with Superconducting Qubits

Youwei Zhao,[1,2,3,*] Yangsen Ye,[1,2,3,*] He-Liang Huang,[1,2,3,*] Yiming Zhang,[1,2,3] Dachao Wu,[1,2,3] Huijie Guan,[1,2,3] Qingling Zhu,[1,2,3] Zuolin Wei,[1,2,3] Tan He,[1,2,3] Sirui Cao,[1,2,3] Fusheng Chen,[1,2,3] Tung-Hsun Chung,[1,2,3] Hui Deng,[1,2,3] Daojin Fan,[1,2,3] Ming Gong,[1,2,3] Cheng Guo,[1,2,3] Shaojun Guo,[1,2,3] Lianchen Han,[1,2,3] Na Li,[1,2,3] Shaowei Li,[1,2,3] Yuan Li,[1,2,3] Futian Liang,[1,2,3] Jin Lin,[1,2,3] Haoran Qian,[1,2,3] Hao Rong,[1,2,3] Hong Su,[1,2,3] Lihua Sun,[1,2,3] Shiyu Wang,[1,2,3] Yulin Wu,[1,2,3] Yu Xu,[1,2,3] Chong Ying,[1,2,3] Jiale Yu,[1,2,3] Chen Zha,[1,2,3] Kaili Zhang,[1,2,3] Yong-Heng Huo,[1,2,3] Chao-Yang Lu,[1,2,3] Cheng-Zhi Peng,[1,2,3] Xiaobo Zhu,[1,2,3] and Jian-Wei Pan[1,2,3]

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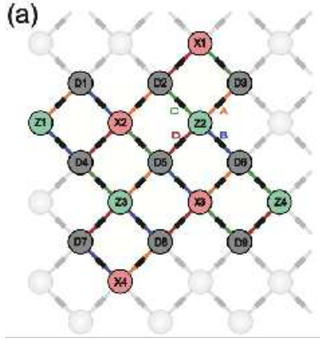
Quantum error correction is a critical technique for transitioning from noisy intermediate-scale quantum (NISQ) devices to fully fledged quantum computers. The surface code, which has a high threshold error rate, is the leading quantum error correction code for two-dimensional grid architecture. So far, the repeated error correction capability of the surface code has not been realized experimentally. Here, we experimentally implement an error-correcting surface code, the distance-3 surface code which consists of 17 qubits, on the *Zuchongzhi* 2.1 superconducting quantum processor. By executing several consecutive error correction cycles, the logical error can be significantly reduced after applying corrections, achieving the repeated error correction of surface code for the first time. This experiment represents a fully functional instance of an error-correcting surface code, providing a key step on the path towards scalable fault-tolerant quantum computing.



Dec 2021

Realizing Repeated Quantum Error Correction in a Distance-Three Surface Code

Sebastian Krinner,[1,*] Nathan Lacroix,[1,*] Ants Remm,[1] Agustin Di Paolo,[2] Elie Genois,[2] Catherine Leroux,[2] Christoph Hellings,[1] Stefania Lazar,[1] Francois Swiadek,[1] Johannes Herrmann,[1] Graham J. Norris,[1] Christian Kraglund Andersen,[1,†] Markus Müller,[3,4] Alexandre Blais,[2,5] Christopher Eichler,[1] and Andreas Wallraff[1,6]

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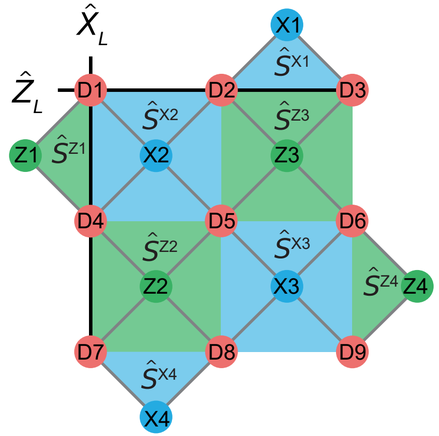
(Dated: December 8, 2021)

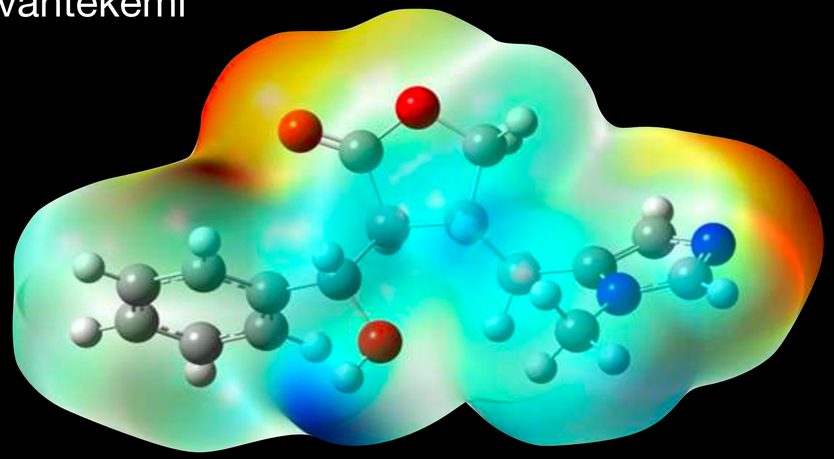
Quantum computers hold the promise of solving computational problems which are intractable using conventional methods [1]. For fault-tolerant operation quantum computers must correct errors occurring due to unavoidable decoherence and limited control accuracy [2]. Here, we demonstrate quantum error correction using the surface code, which is known for its exceptionally high tolerance to errors [3–6]. Using 17 physical qubits in a superconducting circuit, we encode quantum information in a distance-three logical qubit building up on recent distance-two error detection experiments [7–9]. In an error correction cycle taking only 1.1 µs, we demonstrate the preservation of four cardinal states of the logical qubit. Repeatedly executing the cycle, we measure and decode both bit- and phase-flip error syndromes using a minimum-weight perfect-matching algorithm in an error-model-free approach and apply corrections in postprocessing. We find a low error probability of 3 % per cycle when rejecting experimental runs in which leakage is detected. The measured characteristics of our device agree well with a numerical model. Our demonstration of repeated, fast and high-performance quantum error correction cycles, together with recent advances in ion traps [10], support our understanding that fault-tolerant quantum computation will be practically realizable.



Dec 2021

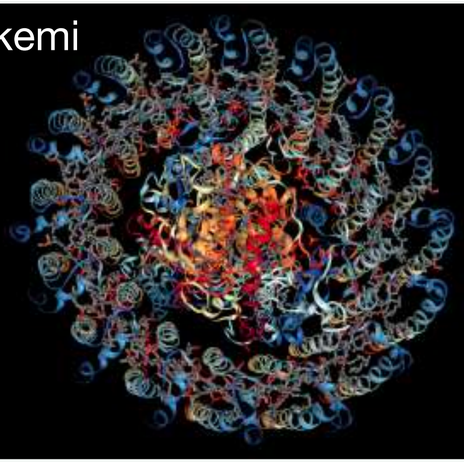
Mere generelt: Hvor forventer vi kvantecomputer ‘speedup’

Kvantekemi



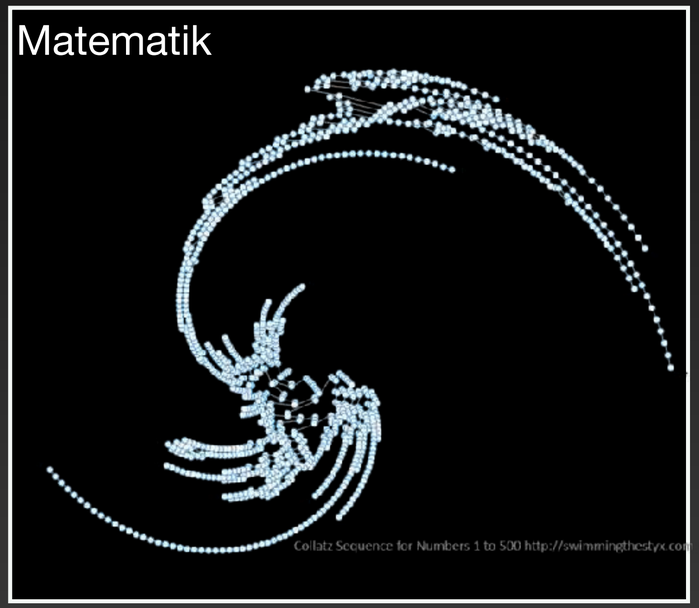
Relevant for kemisk industri/grøn omstilling

Biokemi



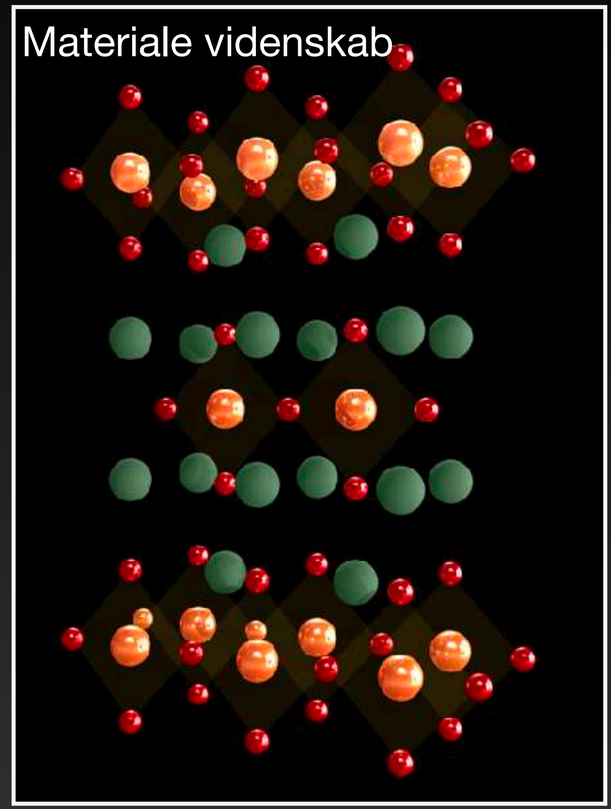
Relevant for life science sektor

Matematik



Relevant for data science/machine learning

Materiale videnskab



Relevant for grøn omstilling

Kemi på en (stor) kvantecomputer

Elucidating reaction mechanisms on quantum computers

Markus Reiher, Nathan Wiebe, Krysta M. Svore, Dave Wecker, and Matthias Troyer
+ See all authors and affiliations

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Edited by David P. DiVincenzo, Institute for Quantum Information, RWTH Aachen University, and accepted by Editorial Board Member Evelyn L. Hu May 24, 2017 (received for review December 31, 2016)

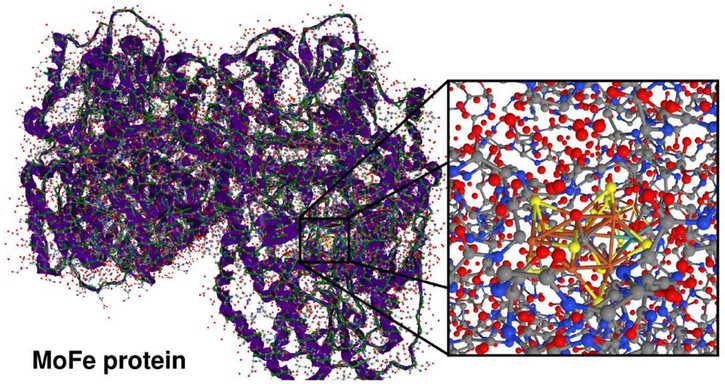
Article | Figures & SI | Info & Metrics | PDF

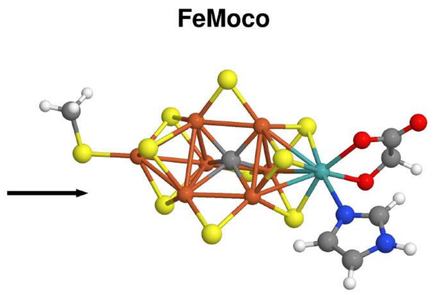
Significance

Our work addresses the question of compelling killer applications for quantum computers. Although quantum chemistry is a strong candidate, the lack of details of how quantum computers can be used for specific applications makes it difficult to assess whether they will be able to deliver on the promises. Here, we show how quantum computers can be used to elucidate the reaction mechanism for biological nitrogen fixation in nitrogenase, by augmenting classical calculation of reaction mechanisms with reliable estimates for relative and activation energies that are beyond the reach of traditional methods. We also show that, taking into account overheads of quantum error correction and gate synthesis, a modular architecture for parallel quantum computers can perform such calculations with components of reasonable complexity.

Table 2. Fault tolerance overheads

Requirements		Serial rotations
Error rate	10^{-3}	10^{-6}
Required code distance	35,17	9
Quantum processor		
Logical qubits	111	111
Physical qubits per logical qubit	15313	1013
Total physical qubits for processor	1.7×10^6	1.1×10^5
Rotation factories		
Number	0	0
Physical qubits per factory	–	–
Total physical qubits for rotations	–	–
T factories		
Number	202	68
Physical qubits per factory	8.7×10^5	1.7×10^4
Total physical qubits for T factories	1.8×10^8	1.1×10^6
Total physical qubits	1.8×10^8	1.2×10^6





PRX QUANTUM **2,** 030305 (2021)

Even More Efficient Quantum Computations of Chemistry Through Tensor Hypercontraction

Joonho Lee,[1,*,§] Dominic W. Berry,[2,†,§] Craig Gidney,[3] William J. Huggins,[3] Jarrod R. McClean,[3] Nathan Wiebe,[4,5] and Ryan Babbush[3,‡]

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We describe quantum circuits with only $\widetilde{\mathcal{O}}(N)$ Toffoli complexity that block encode the spectra of quantum chemistry Hamiltonians in a basis of N arbitrary (e.g., molecular) orbitals. With $\mathcal{O}(\lambda/\epsilon)$ repetitions of these circuits one can use phase estimation to sample in the molecular eigenbasis, where λ is the 1-norm of Hamiltonian coefficients and ϵ is the target precision. This is the lowest complexity shown for quantum computations of chemistry within an arbitrary basis. Furthermore, up to logarithmic factors, this matches the scaling of the most efficient prior block encodings that can work only with orthogonal-basis functions diagonalizing the Coloumb operator (e.g., the plane-wave dual basis). Our key insight is to factorize the Hamiltonian using a method known as tensor hypercontraction (THC) and then to transform the Coulomb operator into an isospectral diagonal form with a nonorthogonal basis defined by the THC factors. We then use qubitization to simulate the nonorthogonal THC Hamiltonian, in a fashion that avoids most complications of the nonorthogonal basis. We also reanalyze and reduce the cost of several of the best prior algorithms for these simulations in order to facilitate a clear comparison to the present work. In addition to having lower asymptotic scaling space-time volume, compilation of our algorithm for challenging finite-sized molecules such as FeMoCo reveals that our method requires the least fault-tolerant resources of any known approach. By laying out and optimizing the surface-code resources required of our approach we show that FeMoCo can be simulated using about four million physical qubits and under 4 days of runtime, assuming 1-μs cycle times and physical gate-error rates no worse than 0.1%.

DOI: 10.1103/PRXQuantum.2.030305

Materialeforskning på en (stor) kvantecomputer

How to simulate key properties of lithium-ion batteries with a fault-tolerant quantum computer

Alain Delgado,[1,*] Pablo A. M. Casares,[2,*] Roberto dos Reis,[1,3] Modjtaba Shokrian Zini,[1] Roberto Campos,[2,4] Norge Cruz-Hernández,[5] Arne-Christian Voigt,[6] Angus Lowe,[1] Soran Jahangiri,[1] M. A. Martin-Delgado,[2,7] Jonathan E. Mueller,[6] and Juan Miguel Arrazola[1,†]

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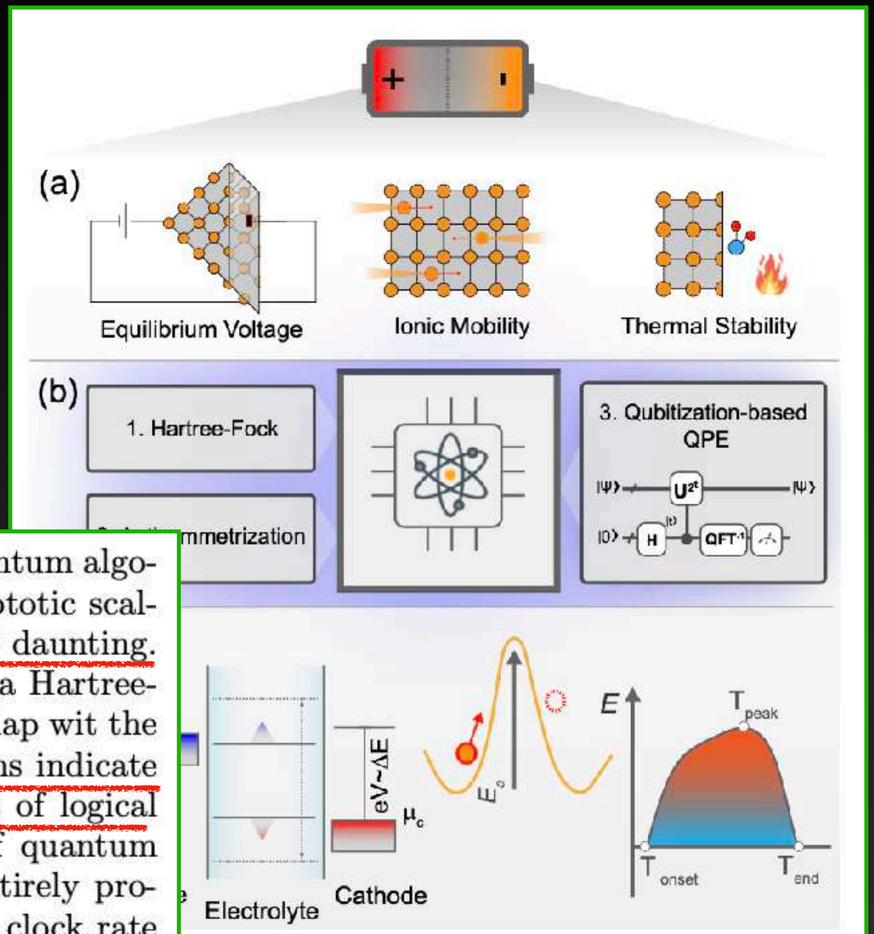
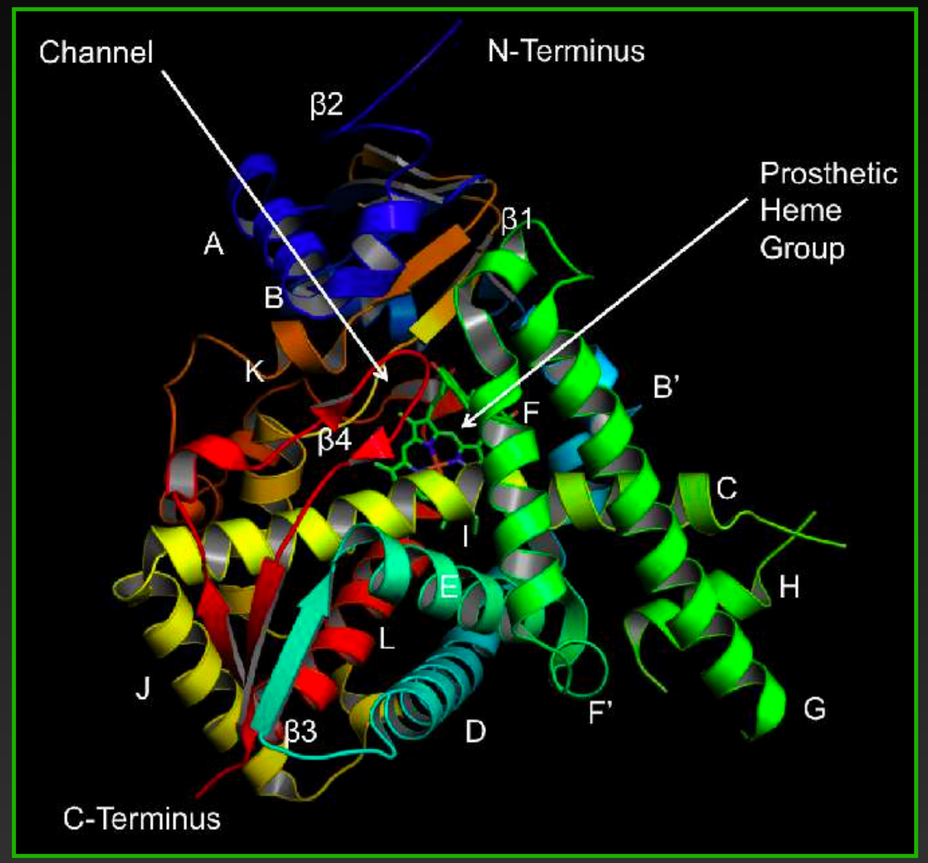
There is a pressing need to develop new rechargeable battery technologies that can offer higher energy storage, faster charging, and lower costs. Despit
simulation of battery materials, they can sometimes fal
results. Quantum computing has been discussed as an
limited work has been done to outline how they may i
we provide a detailed answer to the following question:
simulate key properties of a lithium-ion battery? Based
techniques, we lay out an end-to-end quantum algorithm
ionic mobility, and thermal stability. These can be obtain
which is the core calculation executed by the quantum co
phase estimation. The algorithm includes explicit metho
of periodic materials in first quantization. We bring th
estimation of the resources required to implement a qu
cathode material, dilithium iron silicate.

A careful resource estimation of the full quantum algorithm reveals that despite its favorable asymptotic scaling, the overall resource requirements remain daunting. This is true even under the assumption that a Hartree-Fock approximation has sufficiently large overlap wit the true ground state. Concretely, our calculations indicate that thousands of logical qubits and trillions of logical gates are necessary to execute one round of quantum phase estimation. These numbers are not entirely prohibitive; based on optimistic estimates of the clock rate of fault-tolerant quantum computers, implementing the full quantum phase estimation algorithm may take somewhere between hours to months depending on the number of plane waves used. Nevertheless, these resource estimates are a pressing invitation to undertake a dedicated effort aimed at reducing the cost of the quantum algorithm by many orders of magnitude.



Biotech relevant forskning på en (stor) kvantecomputer



Cytochrome P450

Cytochrome P450 and Chemical Toxicology

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Chem. Res. Toxicol. **2008,** *21,* 70–83

Received March 12, 2007

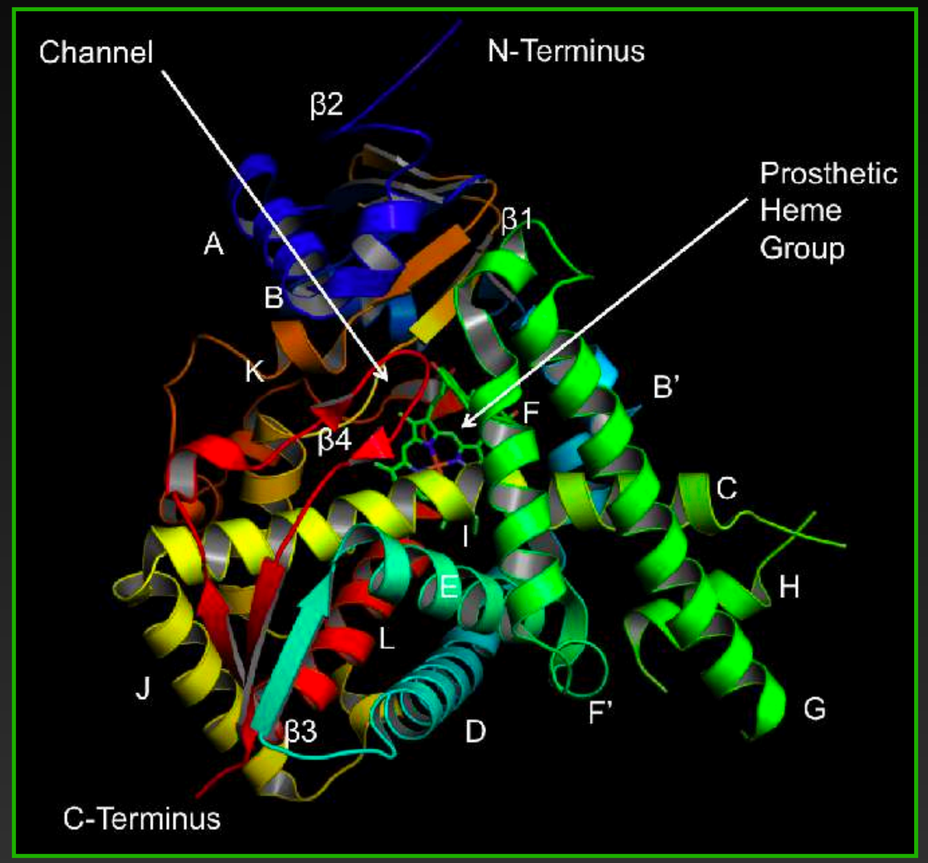
2. Roles of P450s in Reducing Toxicity

P450s are the major enzymes involved in drug metabolism, accounting for ~75% (Figure 4A). Of the 57 human P450s, five are involved in ~95% of the reactions (Figure 4B), which is fortuitous in simplifying the task of assigning new reactions to individual P450s (*57*).

One issue in drug development is bioavailability, and a common initial study is usually "microsomal stability" to predict if most of a drug will be eliminated too rapidly in a "first-pass" effect (*59*). Another issue is side effects due to the inherent pharmacology of the parent drug. Drug doses are adjusted so that most people will clear the drug at a reasonable rate. However, if an individual has an inherent (e.g., genetic) deficiency of a particular P450 or that P450 is inhibited by another drug, toxicity may develop, particularly if drug accumulation occurs upon multiple doses. Drug–drug interactions are recognized to be a major cause of adverse drug reactions.

The field of cytochrome P450 (P450) research has developed considerably over the past 20 years, and many important papers on the roles of P450s in chemical toxicology have appeared in *Chemical Research in Toxicology*. Today, our basic understanding of many of the human P450s is relatively well-established, in terms of the details of the individual genes, sequences, and basic catalytic mechanisms. Crystal structures of several of the major human P450s are now in hand. The animal P450s are still important in the context of metabolism and safety testing. Many well-defined examples exist for roles of P450s in decreasing the adverse effects of drugs through biotransformation, and an equally interesting field of investigation is the bioactivation of chemicals, including drugs. Unresolved problems include the characterization of the minor "orphan" P450s, ligand cooperativity and kinetic complexity of several P450s, the prediction of metabolism, the overall contribution of bioactivation to drug idiosyncratic problems, the extrapolation of animal test results to humans in drug development, and the contribution of genetic variation in human P450s to cancer incidence.

Biotech relevant forskning på en (stor) kvantecomputer



Cytochrome P450

Reliably assessing the electronic structure of cytochrome P450 on today's classical computers and tomorrow's quantum computers

Joshua J. Goings,[1,*] Alec White,[2,*] Joonho Lee,[1,3] Christofer S. Tautermann,[4,5] Matthias Degroote,[6] Craig Gidney,[1] Toru Shiozaki,[2] Ryan Babbush,[1,†] and Nicholas C. Rubin[1,‡]

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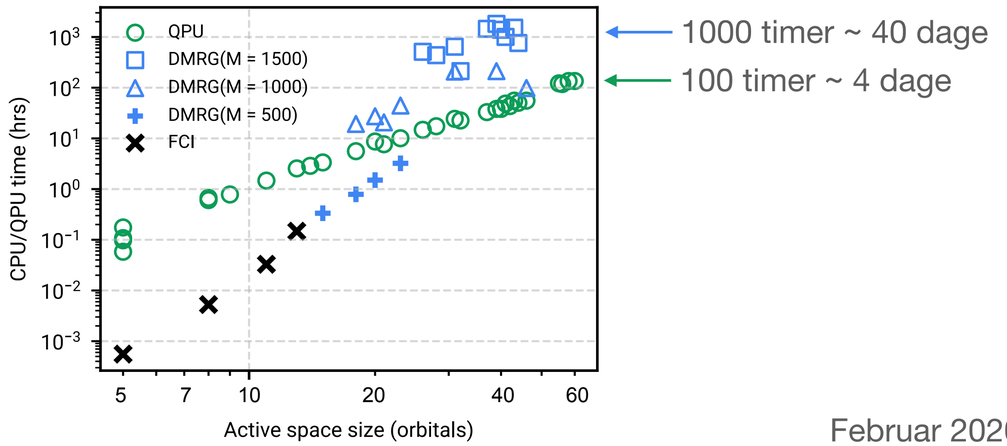
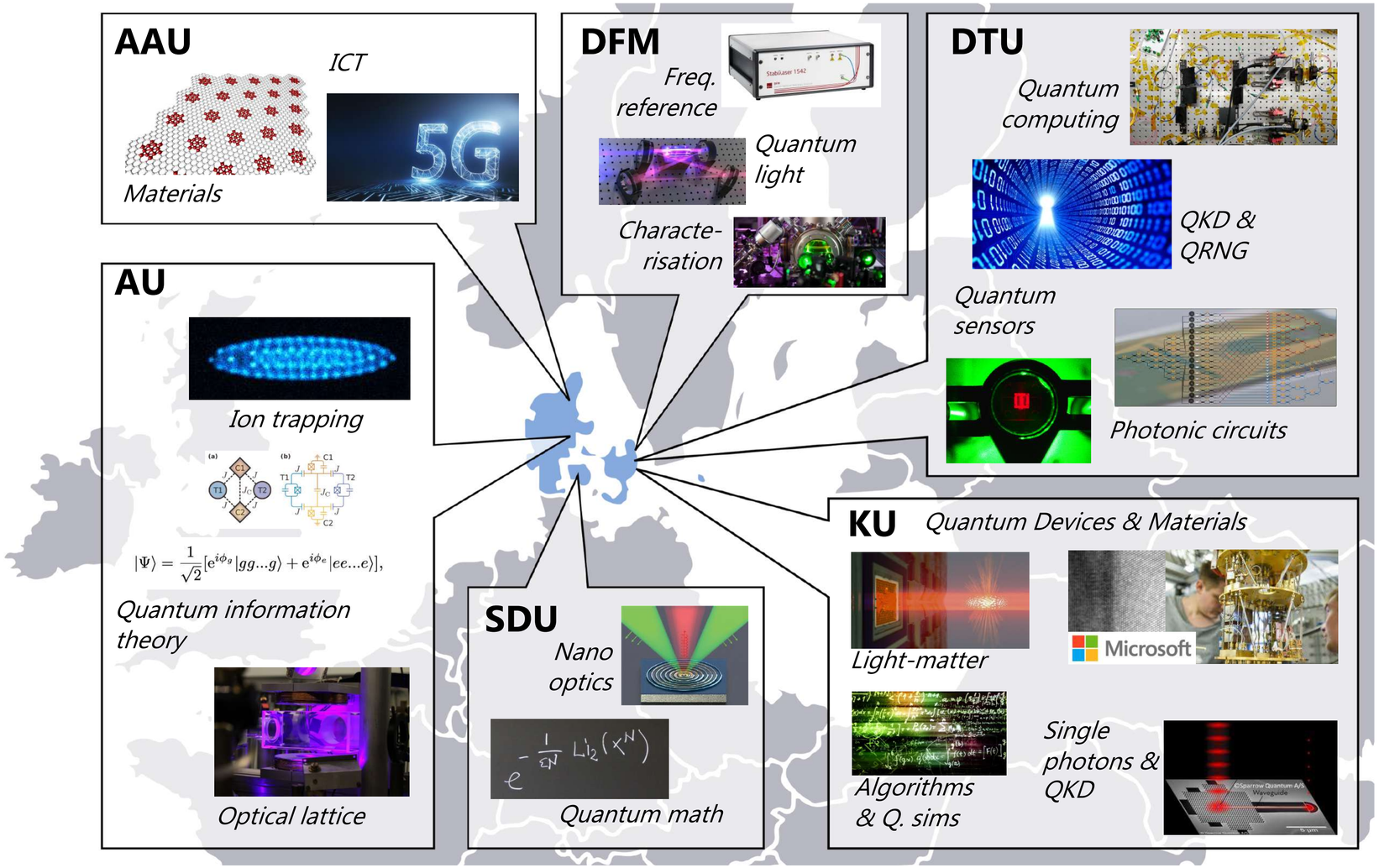
An accurate assessment of how quantum computers can be used for chemical simulation, especially their potential computational advantages, provides important context on how to deploy these future devices. In order to perform this assessment reliably, quantum resource estimates must be coupled with classical simulations attempting to answer relevant chemical questions and to define the classical simulation frontier. Herein, we explore the quantum and classical resources required to assess the electronic structure of cytochrome P450 enzymes (CYPs) and thus define a classical-quantum advantage boundary. This is accomplished by analyzing the convergence of DMRG+NEVPT2 and coupled cluster singles doubles with non-iterative triples (CCSD(T)) calculations for spin-gaps in models of the CYP catalytic cycle that indicate multireference character. The quantum resources required to perform phase estimation using qubitized quantum walks are calculated for the same systems. Compilation into the surface-code provides runtime estimates to compare directly to DMRG runtimes and to evaluate potential quantum advantage. Both classical and quantum resource estimates suggest that simulation of CYP models at scales large enough to balance dynamic and multiconfigurational electron correlation has the potential to be a quantum advantage problem and emphasizes the important interplay between classical simulations and quantum algorithms development for chemical simulation.



Februar 2020

A strong research community

at the international forefront of Quantum Technology



Slide fra Peter Viereck og Danish Quantum Community

Danish quantum industry landscape

Startups and SMEs

CRYPTOMATHIC

SPARROW QUANTUM

NKT Photonics

kvantify

Alea Quantum Technologies

QDevil

SiPhotonIC TECHNOLOGIES

MQS

Global players with quantum activities in Denmark

IBM

KPMG

Microsoft

Ørsted

Slide fra Peter Viereck og Danish Quantum Community

Other Danish stakeholders actively supporting quantum

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Danish National Research Foundation

Innovation Fund Denmark

IT-BRANCHEN

VILLUM FONDEN

Ministry of Higher Education and Science

COPENHAGEN CAPACITY

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MINISTRY OF FOREIGN AFFAIRS OF DENMARK
Invest in Denmark

IDA

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FREMMER DANSK KONKURRENCEEVNE
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Slide fra Peter Viereck og Danish Quantum Community

Center for Quantum Devices

Kvantecomputer udvikling
En opdatering fra frontlinjerne

Tak for opmærksomheden!

Morten Kjaergaard (mkjaergaard@nbi.ku.dk)
Niels Bohr Instituttet

DIREC — IDA — ATV
06/05/2022

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