「次世代計算基盤に係る調査研究 新計算原理チーム報告会」（2024年5月29日、オンライン）

NISQアルゴリズムの最新動向

ー NISQアプリケーションの動向を中心に ー

柚木 清司 (RIKEN)

RIKEN QUANTUM COMPUTING

RIKEN

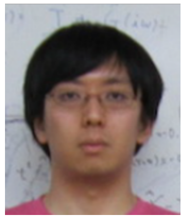
NISQアルゴリズムの最新動向

ー NISQアプリケーションの動向を中心に ー

柚木 清司 (RIKEN)

collaborator:

関 和弘 (RIKEN)



RIKEN QUANTUM COMPUTING

RIKEN

NISQアルゴリズムの最新動向

ー NISQアプリケーションの動向を中心に ー

- NISQコンピュータに関して（early-FTQC & FTQCに関しては谷本チームの報告参照）
- NISQコンピュータ利用・応用の動向
- NISQコンピュータ応用
- NISQコンピュータを実際に利用してみて

RIKEN QUANTUM COMPUTING

RIKEN

NISQコンピュータ利用・応用の動向

arXiv > quant-ph > arXiv:2307.16130

Search...

Help | Adva

Quantum Physics

[Submitted on 30 Jul 2023 (v1), last revised 10 Oct 2023 (this version, v2)]

A comprehensive survey on quantum computer usage: How many qubits are employed for what purposes?

Tsubasa Ichikawa, Hideaki Hakoshima, Koji Inui, Kosuke Ito, Ryo Matsuda, Kosuke Mitarai, Koichi Miyamoto, Wataru Mizukami, Kaoru Mizuta, Toshio Mori, Yuichiro Nakano, Akimoto Nakayama, Ken N. Okada, Takanori Sugimoto, Souichi Takahira, Nayuta Takemori, Satoyuki Tsukano, Hiroshi Ueda, Ryo Watanabe, Yuichiro Yoshida, Keisuke Fujii

Quantum computers (QCs), which work based on the law of quantum mechanics, are expected to be faster than classical computers in several computational tasks such as prime factoring and simulation of quantum many-body systems. In the last decade, research and development of QCs have rapidly advanced. Now hundreds of physical qubits are at our disposal, and one can find several remarkable experiments actually outperforming the classical computer in a specific computational task. On the other hand, it is unclear what the typical usages of the QCs are. Here we conduct an extensive survey on the papers that are posted in the quant-ph section in arXiv and claim to have used QCs in their abstracts. To understand the current situation of the research and development of the QCs, we evaluated the descriptive statistics about the papers, including the number of qubits employed, QPU vendors, application domains and so on. Our survey shows that the annual number of publications is increasing, and the typical number of qubits employed is about six to ten, growing along with the increase in the quantum volume (QV). Most of the preprints are devoted to applications such as quantum machine learning, condensed matter physics, and quantum chemistry, while quantum error correction and quantum noise mitigation use more qubits than the other topics. These imply that the increase in QV is fundamentally relevant, and more experiments for quantum error correction, and noise mitigation using shallow circuits with more qubits will take place.

Comments: 14 pages, 5 figures, figures regenerated
Subjects: **Quantum Physics (quant-ph)**
Cite as: arXiv:2307.16130 **[quant-ph]**
(or arXiv:2307.16130v2 **[quant-ph]** for this version)
https://doi.org/10.48550/arXiv.2307.16130

To be published in Nature Reviews Physics

To be published in **Nature Reviews Physics**

Quantum Physics

[Submitted on 30 Jul 2023 (v1), last revised 10 Oct 2023 (this version, v2)]

A comprehensive survey on quantum computer usage: How many qubits are employed for what purposes?

Tsubasa Ichikawa, Hideaki Hakoshima, Koji Inui, Kosuke Ito, Ryo Matsuda, Kosuke Mitarai, Koichi Miyamoto, Wataru Mizukami, Kaoru Mizuta, Toshio Mori, Yuichiro Nakano, Akimoto Nakayama, Ken N. Okada, Takanori Sugimoto, Souichi Takahira, Nayuta Takemori, Satoyuki Tsukano, Hiroshi Ueda, Ryo Watanabe, Yuichiro Yoshida, Keisuke Fujii

- **2016年1月から2022年11月10日までにarXiv: quant-phに投稿された論文の中で、量子コンピュータ(QC)実機を用いた論文を調査：全748論文**

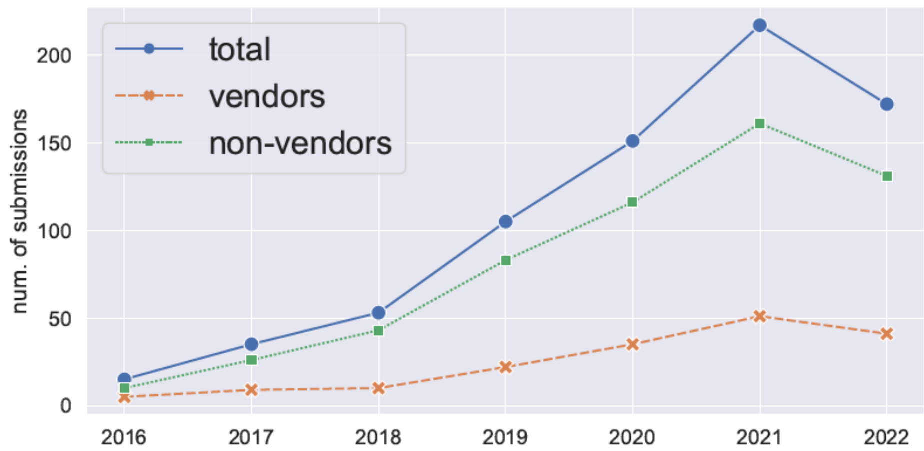
- **量子コンピュータ(QC)実機：Google, IBM, IonQ, Quantinuum, and Rigetti**

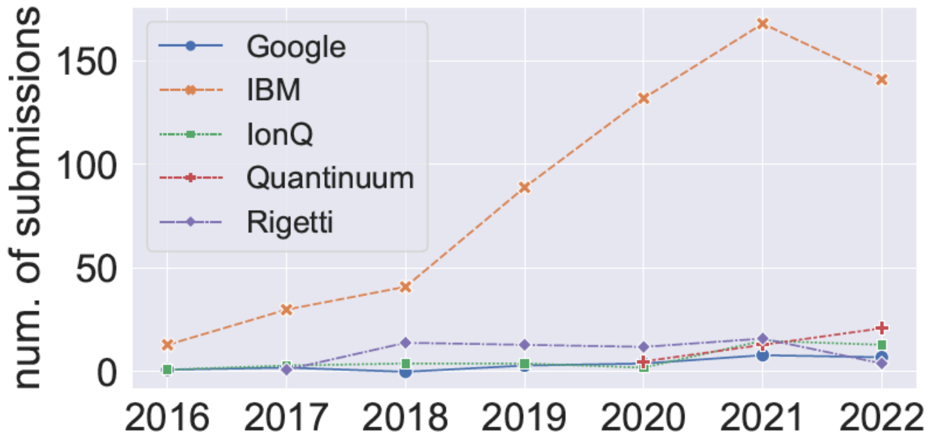
- **2016年1月：IBMがcloud serviceを開始**

- **2017年3月7日：Qiskitをリリース**

T. Ichikawa et al., arXiv:2307.16130 ('23)

- 年別論文数

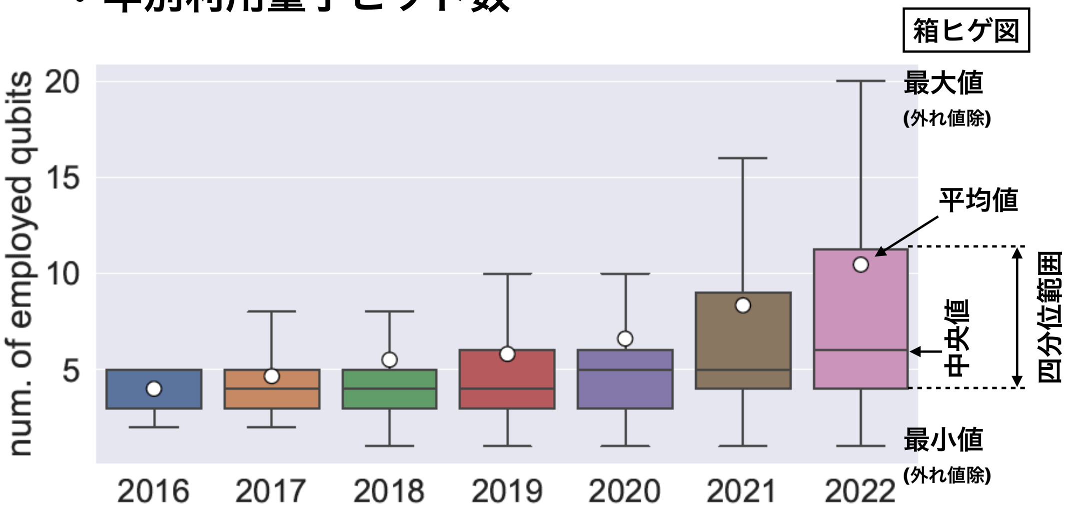


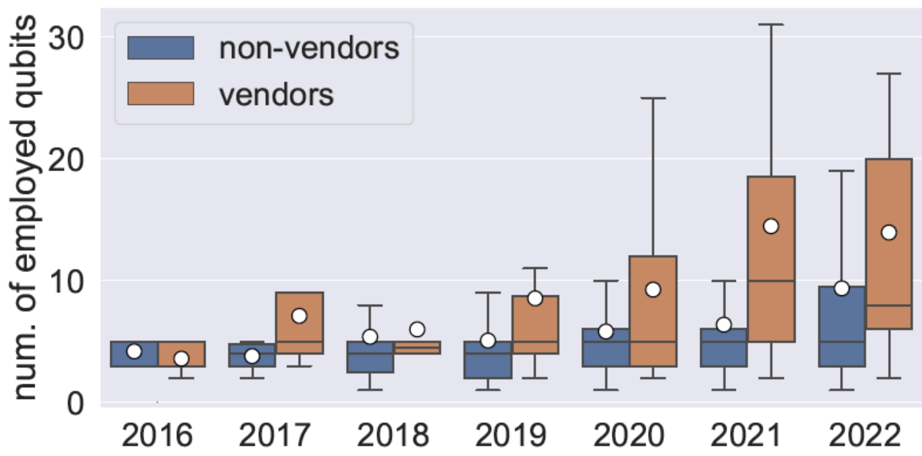


Google: 3.8%
IBM: 75.8%
IonQ: 7.0%
Quantinuum: 11.3%
Rigetti: 2.2%

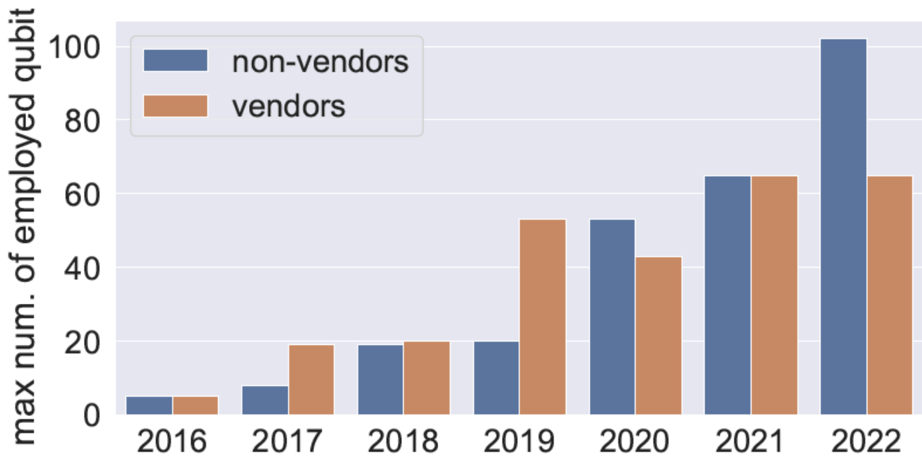
T. Ichikawa et al., arXiv:2307.16130 ('23)

- 年別利用量子ビット数



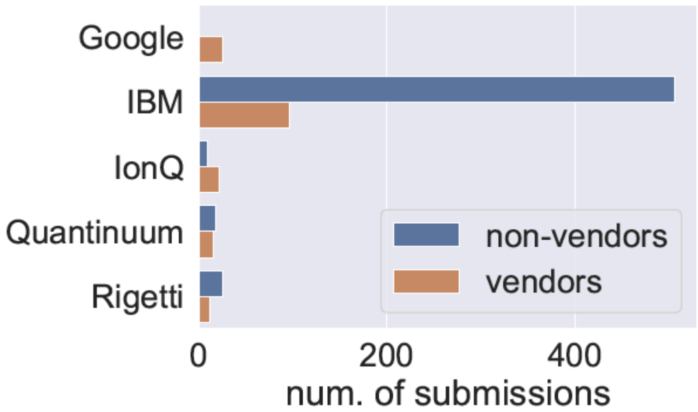


- 年別最大利用量子ビット数

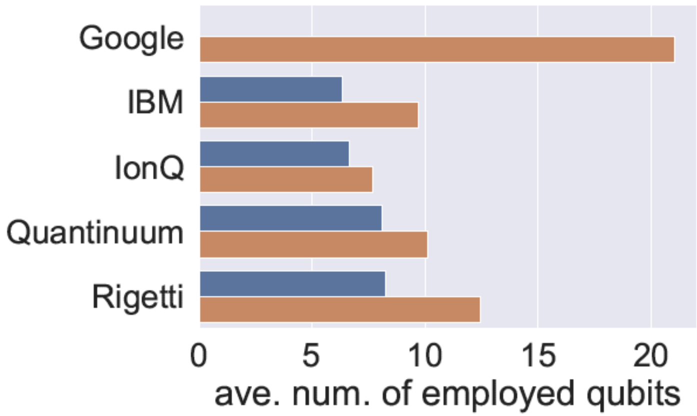


T. Ichikawa et al., arXiv:2307.16130 ('23)

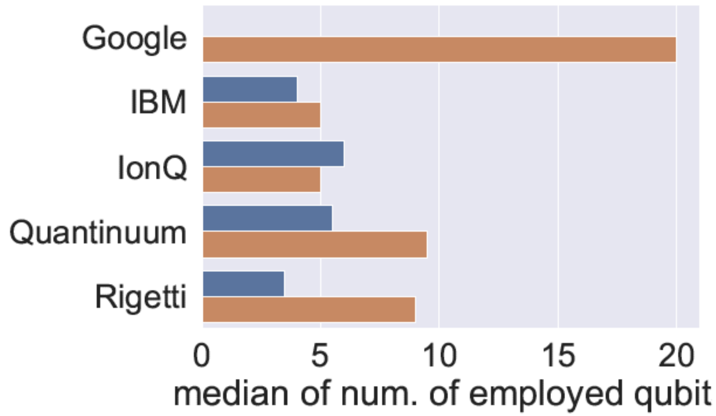
- 全論文数



- 利用量子ビット数 (平均)

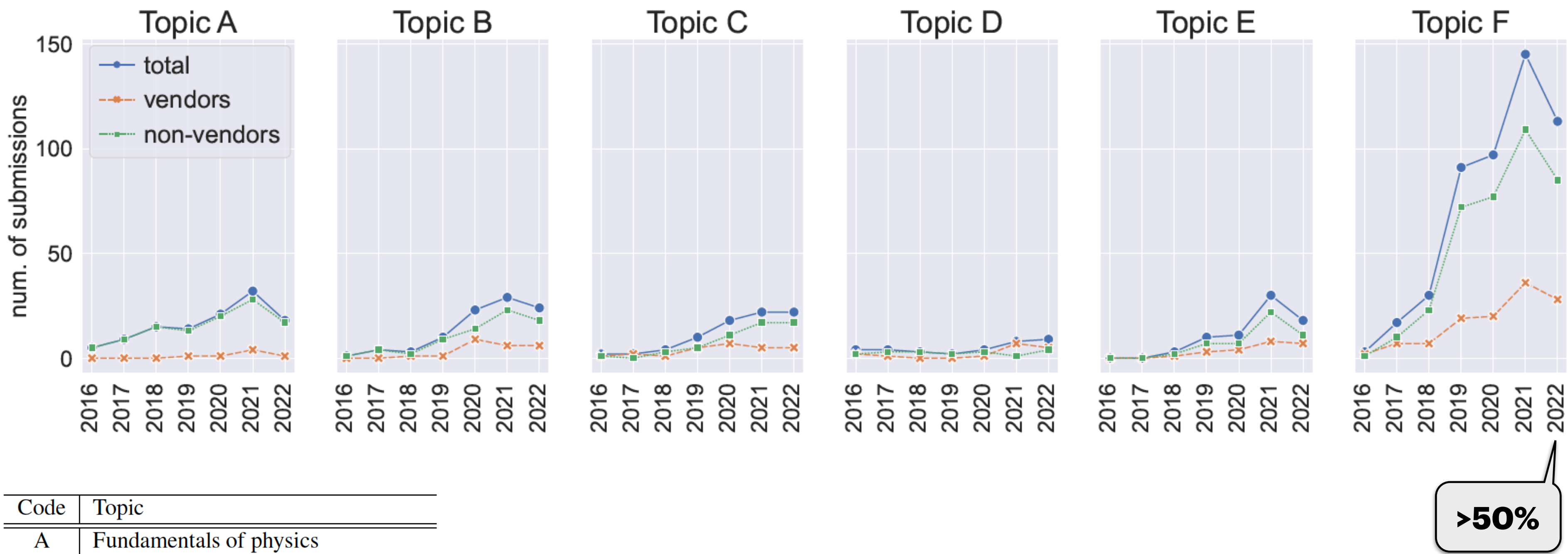


- 利用量子ビット数 (中央値)



T. Ichikawa et al., arXiv:2307.16130 ('23)

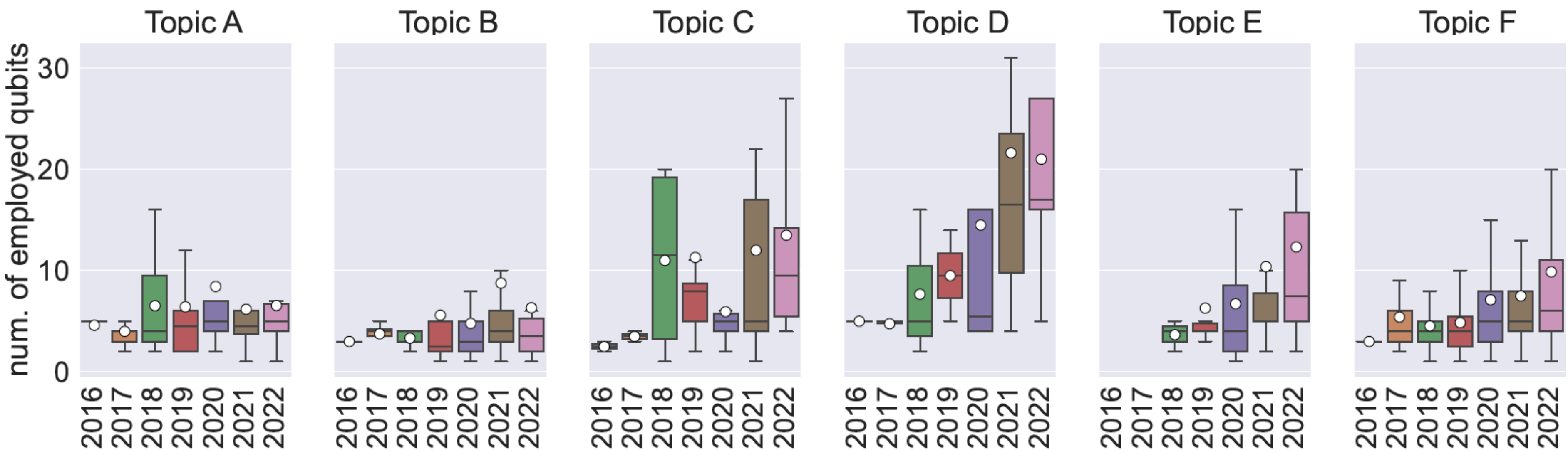
- 利用種別：年別論文数



Code	Topic
A	Fundamentals of physics and quantum information
B	Tomography, noise characterization, quantum control (including pulse optimization), gate benchmarking
C	System and software development for quantum computers
D	Quantum error correction
E	Quantum noise mitigation
F	Applications

T. Ichikawa et al., arXiv:2307.16130 ('23)

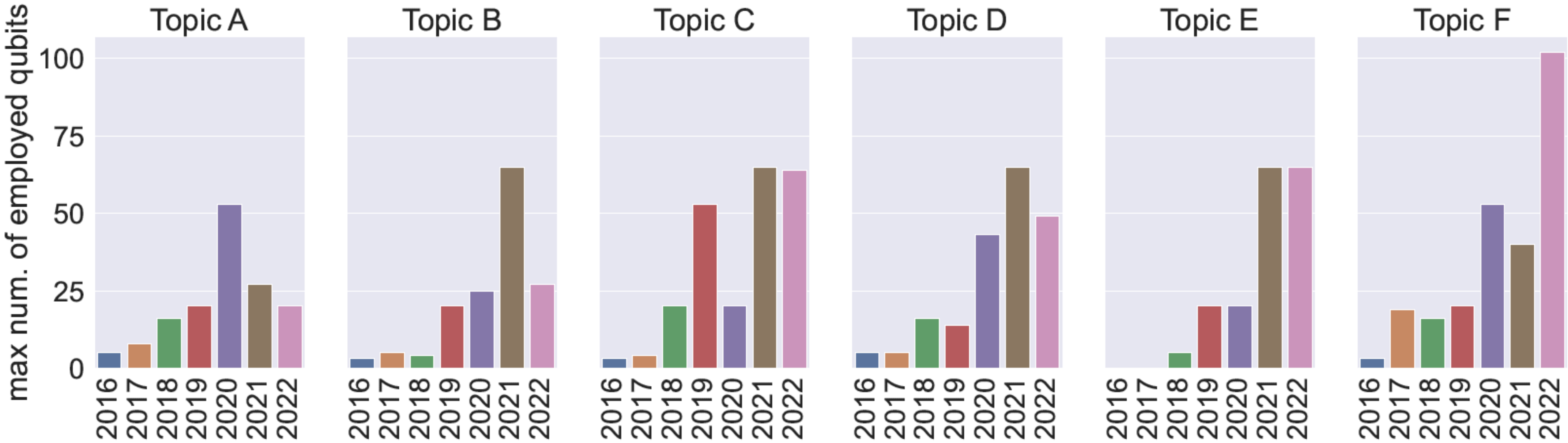
- 利用種別：年別利用量子ビット数



Code	Topic
A	Fundamentals of physics and quantum information
B	Tomography, noise characterization, quantum control (including pulse optimization), gate benchmarking
C	System and software development for quantum computers
D	Quantum error correction
E	Quantum noise mitigation
F	Applications

T. Ichikawa et al., arXiv:2307.16130 ('23)

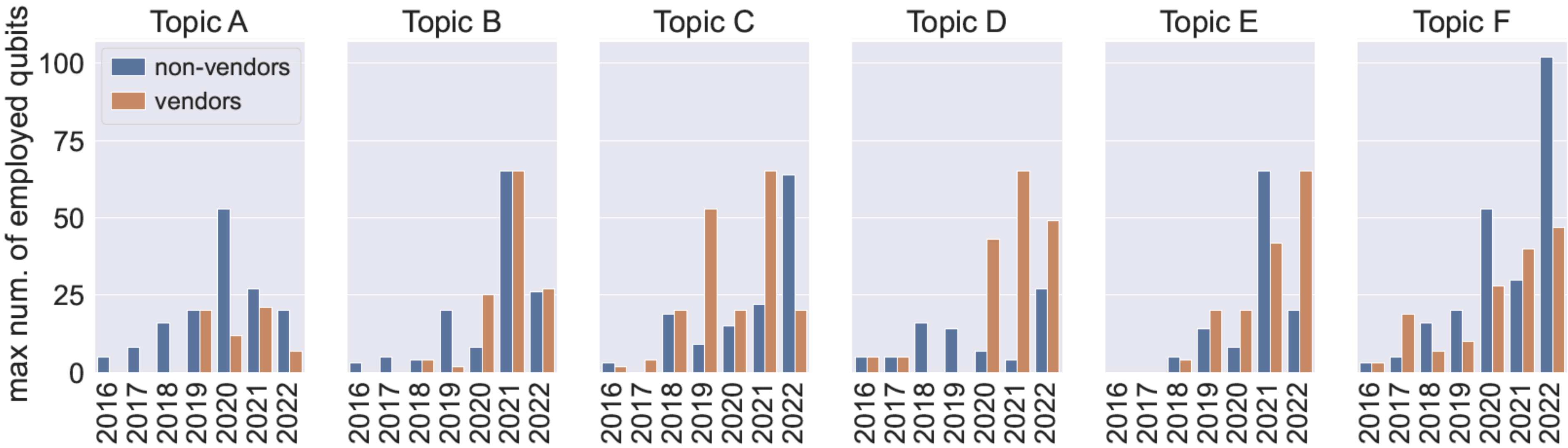
- 利用種別：年別最大利用量子ビット数



Code	Topic
A	Fundamentals of physics and quantum information
B	Tomography, noise characterization, quantum control (including pulse optimization), gate benchmarking
C	System and software development for quantum computers
D	Quantum error correction
E	Quantum noise mitigation
F	Applications

T. Ichikawa et al., arXiv:2307.16130 ('23)

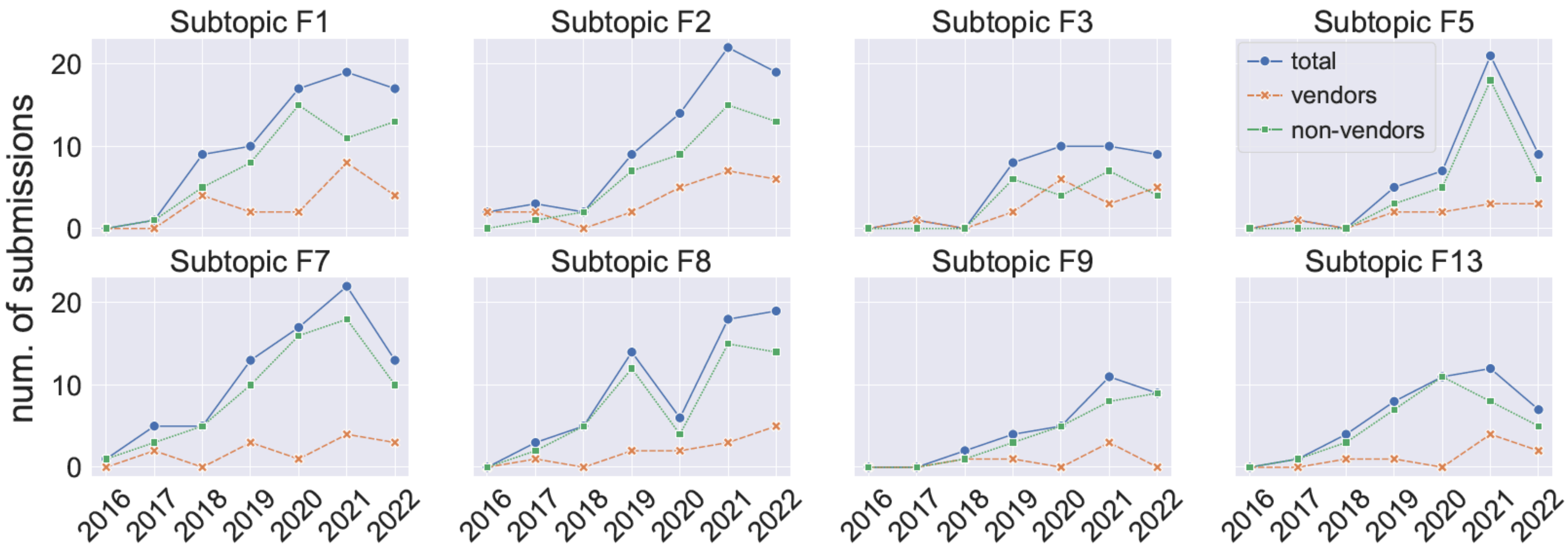
- 利用種別：年別最大利用量子ビット数



Code	Topic
A	Fundamentals of physics and quantum information
B	Tomography, noise characterization, quantum control (including pulse optimization), gate benchmarking
C	System and software development for quantum computers
D	Quantum error correction
E	Quantum noise mitigation
F	Applications

T. Ichikawa et al., arXiv:2307.16130 ('23)

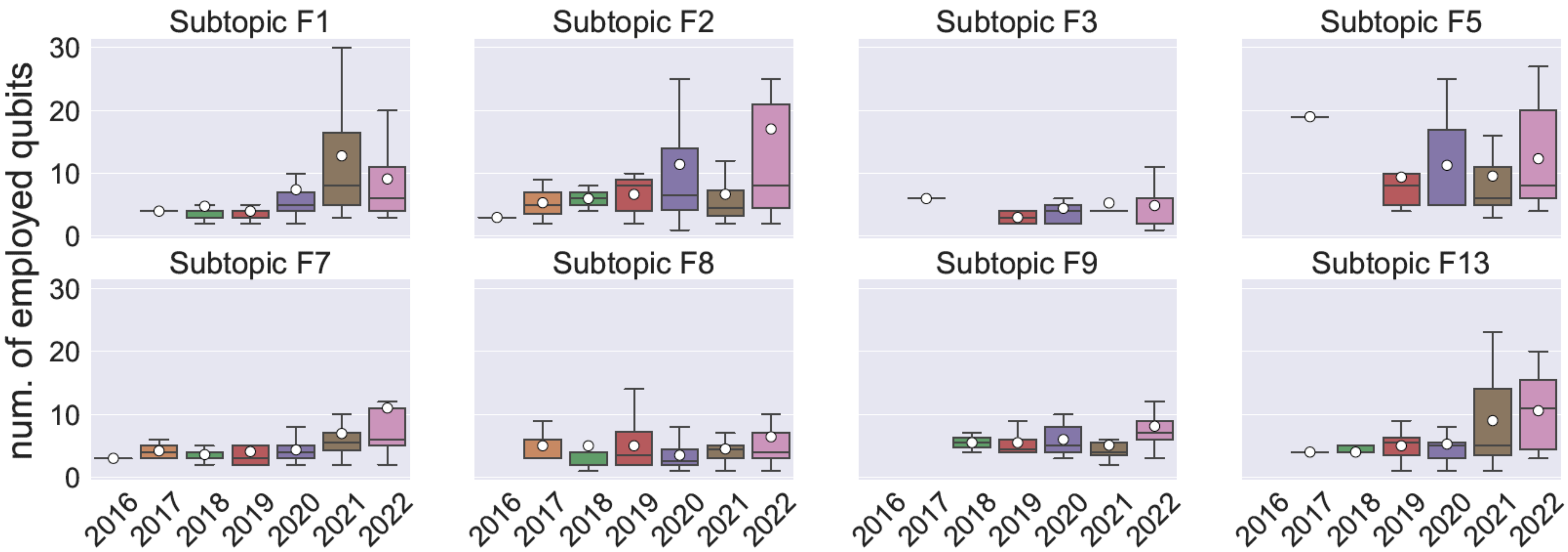
- 「Applications」内訳：年別論文数



Code	Subtopic in F: Applications
F1	Quantum machine learning
F2	Condensed matter physics
F3	Quantum chemistry
F4	Finance
F5	Optimization (QAOA)
F6	Linear algebra (HHL, variational linear system solver)
F7	Primitives (Grover's algorithm, amplitude amplification, phase estimation, variational algorithm, optimizers, measurements)
F8	Simulating quantum mechanics
F9	High energy physics
F10	Fluid dynamics and other differential equations
F11	Open quantum systems
F12	Quantum walk
F13	Others

T. Ichikawa et al., arXiv:2307.16130 ('23)

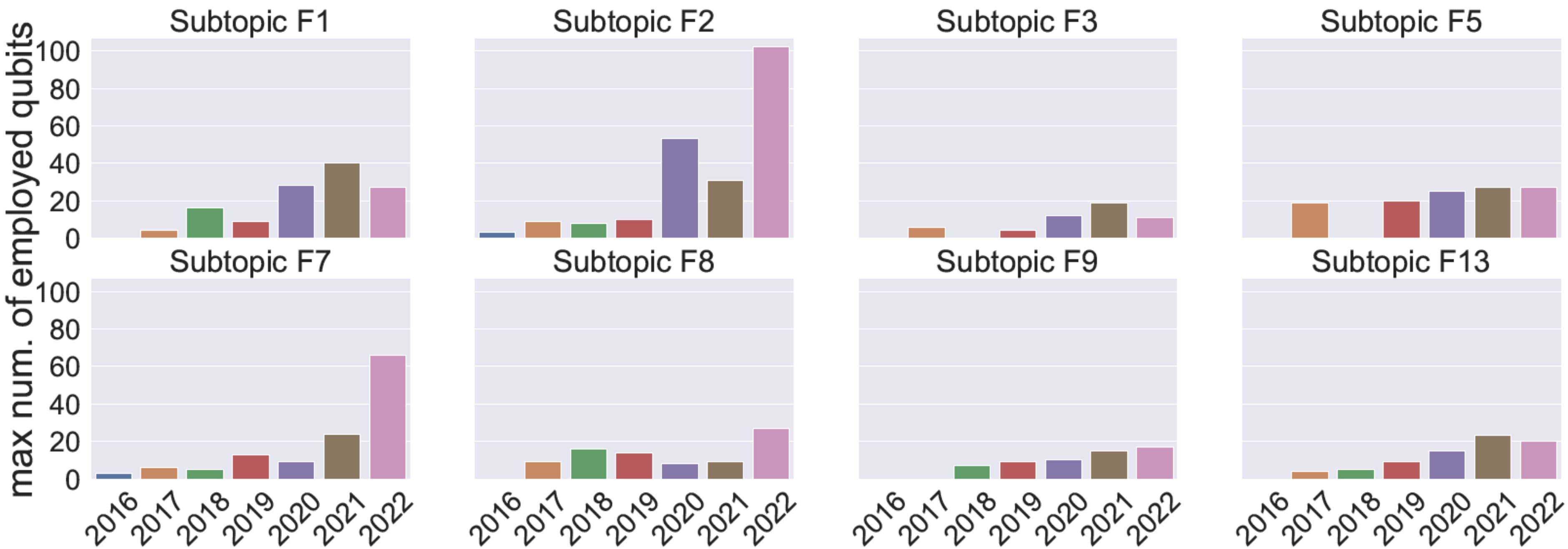
- 「Applications」内訳：年別利用量子ビット数



Code	Subtopic in F: Applications
F1	Quantum machine learning
F2	Condensed matter physics
F3	Quantum chemistry
F4	Finance
F5	Optimization (QAOA)
F6	Linear algebra (HHL, variational linear system solver)
F7	Primitives (Grover's algorithm, amplitude amplification, phase estimation, variational algorithm, optimizers, measurements)
F8	Simulating quantum mechanics
F9	High energy physics
F10	Fluid dynamics and other differential equations
F11	Open quantum systems
F12	Quantum walk
F13	Others

T. Ichikawa et al., arXiv:2307.16130 ('23)

- 「Applications」内訳：年別最大利用量子ビット数



Code	Subtopic in F: Applications
F1	Quantum machine learning
F2	Condensed matter physics
F3	Quantum chemistry
F4	Finance
F5	Optimization (QAOA)
F6	Linear algebra (HHL, variational linear system solver)
F7	Primitives (Grover's algorithm, amplitude amplification, phase estimation, variational algorithm, optimizers, measurements)
F8	Simulating quantum mechanics
F9	High energy physics
F10	Fluid dynamics and other differential equations
F11	Open quantum systems
F12	Quantum walk
F13	Others

To be published in Nature Reviews Physics

arXiv > quant-ph > arXiv:2307.16130

Search...

Help | Adva

Quantum Physics

[Submitted on 30 Jul 2023 (v1), last revised 10 Oct 2023 (this version, v2)]

A comprehensive survey on quantum computer usage: How many qubits are employed for what purposes?

Tsubasa Ichikawa, Hideaki Hakoshima, Koji Inui, Kosuke Ito, Ryo Matsuda, Kosuke Mitarai, Koichi Miyamoto, Wataru Mizukami, Kaoru Mizuta, Toshio Mori, Yuichiro Nakano, Akimoto Nakayama, Ken N. Okada, Takanori Sugimoto, Souichi Takahira, Nayuta Takemori, Satoyuki Tsukano, Hiroshi Ueda, Ryo Watanabe, Yuichiro Yoshida, Keisuke Fujii

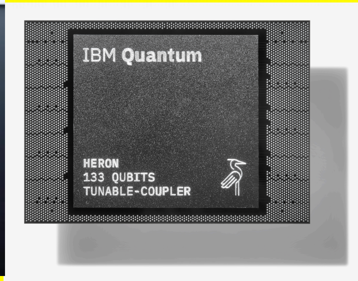
Good practices for use of NISQ computers:

- **Sampling task**
- **Quantum many-body system simulation**
- **Quantum error correction**

Quantum-classical hybrid scheme

quantum computer

IBM **Quantum**



describe a quantum state

classical computer

pre/post processing
less demanding tasks

....

Variational quantum eigenvalue solver (VQE)

A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik & J. L. O'Brien, Nat. Commun. **5**, 4213 ('14)

$$\boxed{\hat{H}|\Psi(\{\theta_i\})\rangle = E(\{\theta_i\})|\Psi(\{\theta_i\})\rangle}$$

variational quantum state:

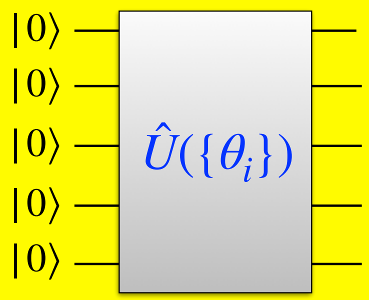
parametrized circuit ansatz

$$|\Psi(\{\theta_i\})\rangle = \hat{U}(\{\theta_i\})|0\rangle =$$

unitary operator

quantum computer

quantum circuit



expectation value of energy

$$E(\{\theta_i\}) = \sum_k \langle \hat{H}_k \rangle_{\{\theta_i\}}$$

$$\hat{H} = \sum_{k=1}^{M} \hat{H}_k$$

classical computer

optimization of variational parameters $\{\theta_i\}$

$$\theta_i \leftarrow \theta_i - \lambda \partial E(\{\theta_i\})/\partial \theta_i$$

N: number of qubits

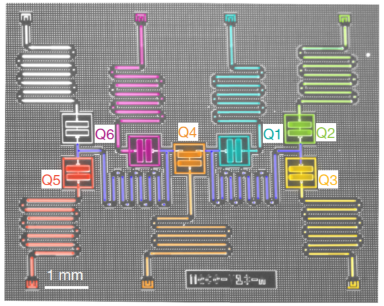
$|\Psi(\{\theta_i\})\rangle$: 2^N dimensional vector
(variational state)

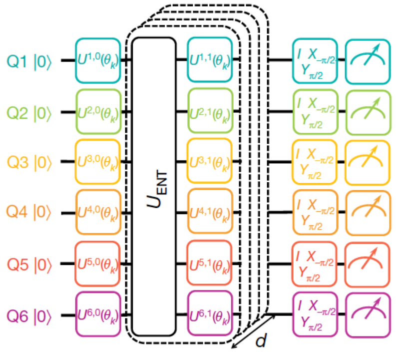
$\{\theta_i\}$: poly(N) dimensional vector
(variational parameters)

Efficient parametrization of a variational state is crucial

Hardware efficient VQE by IBM

A. Kandala, A. Mezzacapo, K. Temme, M. Takita, M. Brink, J. M. Chow & J. M. Gambetta, Nature **549**, 242 ('17)





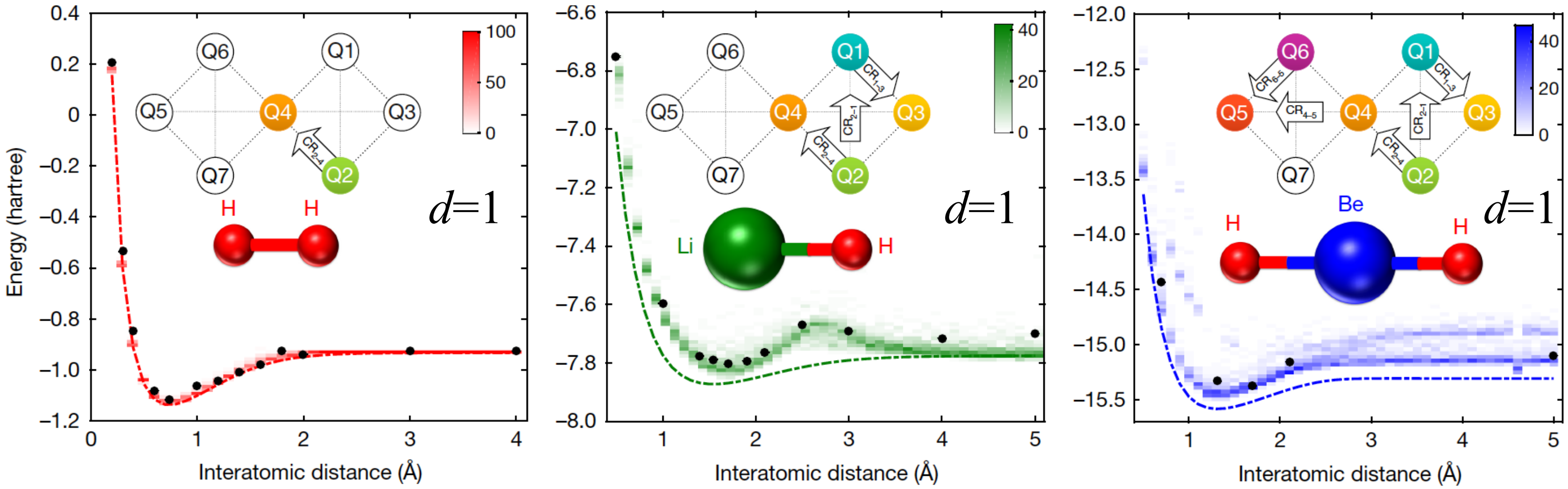
$$|\Phi(\boldsymbol{\theta})\rangle = \prod_{q=1}^{N} [U^{q,d}(\boldsymbol{\theta})] \times U_{\mathrm{ENT}} \times \prod_{q=1}^{N} [U^{q,d-1}(\boldsymbol{\theta})] \times \cdots \times U_{\mathrm{ENT}} \times \prod_{q=1}^{N} [U^{q,0}(\boldsymbol{\theta})] |00\ldots0\rangle$$

U_{ENT}: cross resonance gates that can realize $[ZX]^b$

cf. CNOT=$[ZI]^{-1/2}[ZX]^{1/2}[IX]^{-1/2}$

($[ZX]^{1/2}$ sandwiched by single-qubit rotations)

Rigetti and Devoret, PRB '10



d: number of layers in the circuit

Quantum-centric supercomputing

arXiv > quant-ph > arXiv:2312.09733

Search...

Help | Adva

Quantum Physics

[Submitted on 14 Dec 2023]

Quantum-centric Supercomputing for Materials Science: A Perspective on Challenges and Future Directions

Yuri Alexeev, Maximilian Amsler, Paul Baity, Marco Antonio Barroca, Sanzio Bassini, Torey Battelle, Daan Camps, David Casanova, Young jai Choi, Frederic T. Chong, Charles Chung, Chris Codella, Antonio D. Corcoles, James Cruise, Alberto Di Meglio, Jonathan Dubois, Ivan Duran, Thomas Eckl, Sophia Economou, Stephan Eidenbenz, Bruce Elmegreen, Clyde Fare, Ismael Faro, Cristina Sanz Fernández, Rodrigo Neumann Barros Ferreira, Keisuke Fuji, Bryce Fuller, Laura Gagliardi, Giulia Galli, Jennifer R. Glick, Isacco Gobbi, Pranav Gokhale, Salvador de la Puente Gonzalez, Johannes Greiner, Bill Gropp, Michele Grossi, Emmanuel Gull, Burns Healy, Benchen Huang, Travis S. Humble, Nobuyasu Ito, Artur F. Izmaylov, Ali Javadi-Abhari, Douglas Jennewein, Shantenu Jha, Liang Jiang, Barbara Jones, Wibe Albert de Jong, Petar Jurcevic, William Kirby, Stefan Kister, Masahiro Kitagawa, Joel Klassen, Katherine Klymko, Kwangwon Koh, Masaaki Kondo, Doga Murat Kurkcuoglu, Krzysztof Kurowski, Teodoro Laino, Ryan Landfield, Matt Leininger, Vicente Leyton-Ortega, Ang Li, Meifeng Lin, Junyu Liu, Nicolas Lorente, Andre Luckow, Simon Martiel, Francisco Martin-Fernandez, Margaret Martonosi, Claire Marvinney, Arcesio Castaneda Medina, Dirk Merten, Antonio Mezzacapo, Kristel Michielsen, Abhishek Mitra, Tushar Mittal, Kyungsun Moon, Joel Moore, Mario Motta, Young-Hye Na, Yunseong Nam, Prineha Narang, Yu-ya Ohnishi, Daniele Ottaviani, Matthew Otten, Scott Pakin, Vincent R. Pascuzzi, Ed Penault, Tomasz Piontek, Jed Pitera, Patrick Rall, Gokul Subramanian Ravi, Niall Robertson, Matteo Rossi, Piotr Rydlichowski, Hoon Ryu, Georgy Samsonidze, Mitsuhisa Sato, Nishant Saurabh , Vidushi Sharma, Kunal Sharma, Soyoung Shin, George Slessman, Mathias Steiner, Iskandar Sitdikov, In-Saeng Suh, Eric Switzer, Wei Tang, Joel Thompson, Synge Todo, Minh Tran, Dimitar Trenev, Christian Trott, Huan-Hsin Tseng, Esin Tureci, David García Valinas, Sofia Vallecorsa, Christopher Wever, Konrad Wojciechowski, Xiaodi Wu, Shinjae Yoo, Nobuyuki Yoshioka, Victor Wen-zhe Yu, Seiji Yunoki, Sergiy Zhuk, Dmitry Zubarev (collapse list)

Computational models are an essential tool for the design, characterization, and discovery of novel materials. Hard computational tasks in materials science stretch the limits of existing high-performance supercomputing centers, consuming much of their simulation, analysis, and data resources. Quantum computing, on the other hand, is an emerging technology with the potential to accelerate many of the computational tasks needed for materials science. In order to do that, the quantum technology must interact with conventional high-performance computing in several ways: approximate results validation, identification of hard problems, and synergies in quantum-centric supercomputing. In this paper, we provide a perspective on how quantum-centric supercomputing can help address critical computational problems in materials science, the challenges to face in order to solve representative use cases, and new suggested directions.

Comments: 60 pages, 14 figures; comments welcome
Subjects: **Quantum Physics (quant-ph)**; Materials Science (cond-mat.mtrl-sci)
Cite as: arXiv:2312.09733 **[quant-ph]**
(or arXiv:2312.09733v1 **[quant-ph]** for this version)
https://doi.org/10.48550/arXiv.2312.09733

materials science

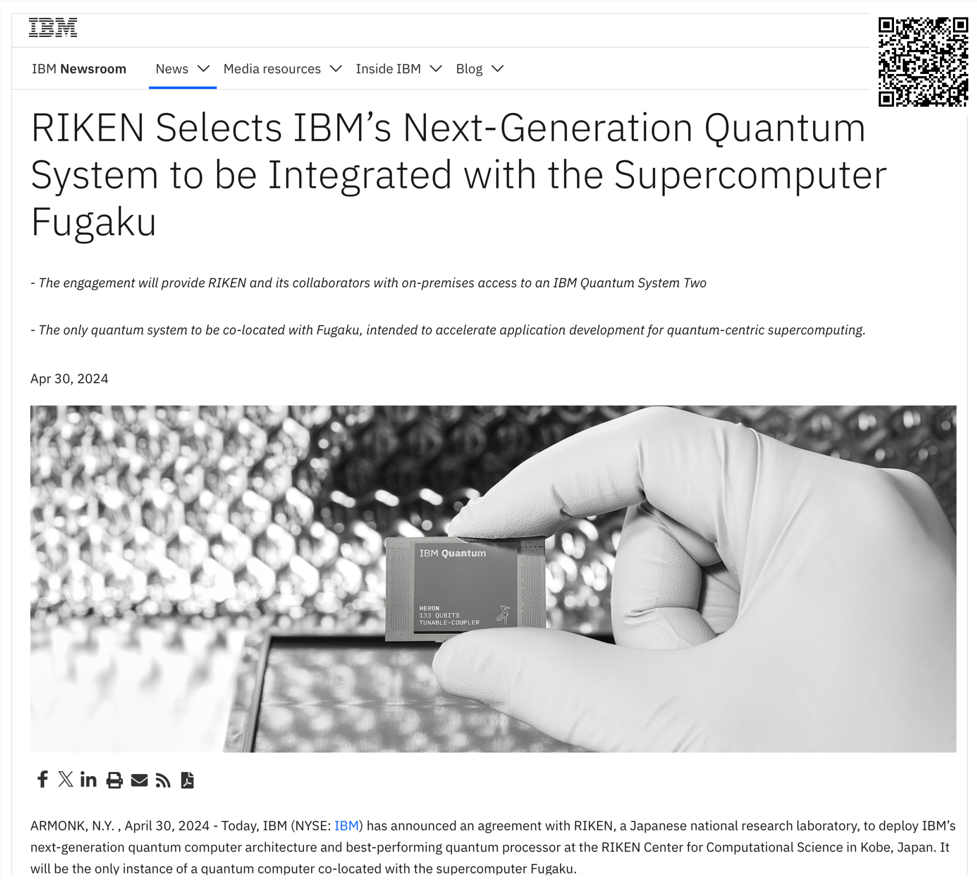
Towards Quantum-Centric Supercomputing

IBM and Riken agree to collaborate for constructing a quantum-HPC hybrid computing system in Riken @ Kobe

■ **JHPC-quantum project:**
"計算可能領域の開拓のための量子・スパコン連携プラットフォームの研究開発", NEDO
(2023/11~2028/10)

JHPC-quantum

M. Sato
(R-CCS)


IBM

IBM Newsroom News Media resources Inside IBM Blog

RIKEN Selects IBM's Next-Generation Quantum System to be Integrated with the Supercomputer Fugaku

- The engagement will provide RIKEN and its collaborators with on-premises access to an IBM Quantum System Two

- The only quantum system to be co-located with Fugaku, intended to accelerate application development for quantum-centric supercomputing.

Apr 30, 2024

ARMONK, N.Y. , April 30, 2024 - Today, IBM (NYSE: IBM) has announced an agreement with RIKEN, a Japanese national research laboratory, to deploy IBM's next-generation quantum computer architecture and best-performing quantum processor at the RIKEN Center for Computational Science in Kobe, Japan. It will be the only instance of a quantum computer co-located with the supercomputer Fugaku.

RIKEN Center for Computational Science @ Kobe

R-CCS

IBM Quantum System Two

×

富岳 Fugaku

arXiv > quant-ph > arXiv:2405.05068

Search...

Help | Adva

Quantum Physics

IBM Quantum

RIKEN

[Submitted on 8 May 2024]

Chemistry Beyond Exact Solutions on a Quantum-Centric Supercomputer

Javier Robledo-Moreno, Mario Motta, Holger Haas, Ali Javadi-Abhari, Petar Jurcevic, William Kirby, Simon Martiel, Kunal Sharma, Sandeep Sharma, Tomonori Shirakawa, Iskandar Sitdikov, Rong-Yang Sun, Kevin J. Sung, Maika Takita, Minh C. Tran, Seiji Yunoki, Antonio Mezzacapo

A universal quantum computer can be used as a simulator capable of predicting properties of diverse quantum systems. Electronic structure problems in chemistry offer practical use cases around the hundred-qubit mark. This appears promising since current quantum processors have reached these sizes. However, mapping these use cases onto quantum computers yields deep circuits, and for for pre-fault-tolerant quantum processors, the large number of measurements to estimate molecular energies leads to prohibitive runtimes. As a result, realistic chemistry is out of reach of current quantum computers in isolation. A natural question is whether classical distributed computation can relieve quantum processors from parsing all but a core, intrinsically quantum component of a chemistry workflow. Here, we incorporate quantum computations of chemistry in a quantum-centric supercomputing architecture, using up to 6400 nodes of the supercomputer Fugaku to assist a Heron superconducting quantum processor. We simulate the N_2 triple bond breaking in a correlation-consistent cc-pVDZ basis set, and the active-space electronic structure of [2Fe-2S] and [4Fe-4S] clusters, using 58, 45 and 77 qubits respectively, with quantum circuits of up to 10570 (3590 2-qubit) quantum gates. We obtain our results using a class of quantum circuits that approximates molecular eigenstates, and a hybrid estimator. The estimator processes quantum samples, produces upper bounds to the ground-state energy and wavefunctions supported on a polynomial number of states. This guarantees an unconditional quality metric for quantum advantage, certifiable by classical computers at polynomial cost. For current error rates, our results show that classical distributed computing coupled to quantum processors can produce good approximate solutions for practical problems beyond sizes amenable to exact diagonalization.

富岳

Fugaku

Subjects: **Quantum Physics (quant-ph)**; Other Condensed Matter (cond-mat.other); Chemical Physics (physics.chem-ph); Computational Physics (physics.comp-ph)

Cite as: arXiv:2405.05068 **[quant-ph]**
(or arXiv:2405.05068v1 **[quant-ph]** for this version)
https://doi.org/10.48550/arXiv.2405.05068

First example of "Quantum-Centric Supercomputing"

Quantum computing for high energy physics

arXiv > quant-ph > arXiv:2307.03236

Search...

Help | Advan

Quantum Physics

[Submitted on 6 Jul 2023]

Quantum Computing for High-Energy Physics: State of the Art and Challenges. Summary of the QC4HEP Working Group

Alberto Di Meglio, Karl Jansen, Ivano Tavernelli, Constantia Alexandrou, Srinivasan Arunachalam, Christian W. Bauer, Kerstin Borras, Stefano Carrazza, Arianna Crippa, Vincent Croft, Roland de Putter, Andrea Delgado, Vedran Dunjko, Daniel J. Egger, Elias Fernandez-Combarro, Elina Fuchs, Lena Funcke, Daniel Gonzalez-Cuadra, Michele Grossi, Jad C. Halimeh, Zoe Holmes, Stefan Kuhn, Denis Lacroix, Randy Lewis, Donatella Lucchesi, Miriam Lucio Martinez, Federico Meloni, Antonio Mezzacapo, Simone Montangero, Lento Nagano, Voica Radescu, Enrique Rico Ortega, Alessandro Roggero, Julian Schuhmacher, Joao Seixas, Pietro Silvi, Panagiotis Spentzouris, Francesco Tacchino, Kristan Temme, Koji Terashi, Jordi Tura, Cenk Tuysuz, Sofia Vallecorsa, Uwe-Jens Wiese, Shinjae Yoo, Jinglei Zhang

Quantum computers offer an intriguing path for a paradigmatic change of computing in the natural sciences and beyond, with the potential for achieving a so-called quantum advantage, namely a significant (in some cases exponential) speed-up of numerical simulations. The rapid development of hardware devices with various realizations of qubits enables the execution of small scale but representative applications on quantum computers. In particular, the high-energy physics community plays a pivotal role in accessing the power of quantum computing, since the field is a driving source for challenging computational problems. This concerns, on the theoretical side, the exploration of models which are very hard or even impossible to address with classical techniques and, on the experimental side, the enormous data challenge of newly emerging experiments, such as the upgrade of the Large Hadron Collider. In this roadmap paper, led by CERN, DESY and IBM, we provide the status of high-energy physics quantum computations and give examples for theoretical and experimental target benchmark applications, which can be addressed in the near future. Having the IBM 100 x 100 challenge in mind, where possible, we also provide resource estimates for the examples given using error mitigated quantum computing.

Subjects: **Quantum Physics (quant-ph)**; High Energy Physics - Experiment (hep-ex); High Energy Physics - Lattice (hep-lat); High Energy Physics - Theory (hep-th)

Cite as: arXiv:2307.03236 **[quant-ph]**
(or arXiv:2307.03236v1 **[quant-ph]** for this version)
https://doi.org/10.48550/arXiv.2307.03236

Submission history

From: Alberto Di Meglio [view email]
[v1] Thu, 6 Jul 2023 18:01:02 UTC (652 KB)

high energy physics

Quantum optimization

arXiv > quant-ph > arXiv:2312.02279

Search...

Help | Advan

Quantum Physics

[Submitted on 4 Dec 2023]

Quantum Optimization: Potential, Challenges, and the Path Forward

Amira Abbas, Andris Ambainis, Brandon Augustino, Andreas Bärtschi, Harry Buhrman, Carleton Coffrin, Giorgio Cortiana, Vedran Dunjko, Daniel J. Egger, Bruce G. Elmegreen, Nicola Franco, Filippo Fratini, Bryce Fuller, Julien Gacon, Constantin Gonciulea, Sander Gribling, Swati Gupta, Stuart Hadfield, Raoul Heese, Gerhard Kircher, Thomas Kleinert, Thorsten Koch, Georgios Korpas, Steve Lenk, Jakub Marecek, Vanio Markov, Guglielmo Mazzola, Stefano Mensa, Naeimeh Mohseni, Giacomo Nannicini, Corey O'Meara, Elena Peña Tapia, Sebastian Pokutta, Manuel Proissl, Patrick Rebentrost, Emre Sahin, Benjamin C. B. Symons, Sabine Tornow, Victor Valls, Stefan Woerner, Mira L. Wolf-Bauwens, Jon Yard, Sheir Yarkoni, Dirk Zechiel, Sergiy Zhuk, Christa Zoufal

Recent advances in quantum computers are demonstrating the ability to solve problems at a scale beyond brute force classical simulation. As such, a widespread interest in quantum algorithms has developed in many areas, with optimization being one of the most pronounced domains. Across computer science and physics, there are a number of algorithmic approaches, often with little linkage. This is further complicated by the fragmented nature of the field of mathematical optimization, where major classes of optimization problems, such as combinatorial optimization, convex optimization, non-convex optimization, and stochastic extensions, have devoted communities. With these aspects in mind, this work draws on multiple approaches to study quantum optimization. Provably exact versus heuristic settings are first explained using computational complexity theory - highlighting where quantum advantage is possible in each context. Then, the core building blocks for quantum optimization algorithms are outlined to subsequently define prominent problem classes and identify key open questions that, if answered, will advance the field. The effects of scaling relevant problems on noisy quantum devices are also outlined in detail, alongside meaningful benchmarking problems. We underscore the importance of benchmarking by proposing clear metrics to conduct appropriate comparisons with classical optimization techniques. Lastly, we highlight two domains - finance and sustainability - as rich sources of optimization problems that could be used to benchmark, and eventually validate, the potential real-world impact of quantum optimization.

Comments: 70 pages, 9 Figures, 4 Tables
Subjects: **Quantum Physics (quant-ph)**; Optimization and Control (math.OC)
Cite as: arXiv:2312.02279 **[quant-ph]**
(or arXiv:2312.02279v1 **[quant-ph]** for this version)
https://doi.org/10.48550/arXiv.2312.02279

quantum optimization

Quantum-enabled cell-centric therapeutics

arXiv > quant-ph > arXiv:2307.05734

Search...

Help | Advanc

Quantum Physics

[Submitted on 11 Jul 2023 (v1), last revised 1 Aug 2023 (this version, v2)]

Towards quantum-enabled cell-centric therapeutics

Saugata Basu, Jannis Born, Aritra Bose, Sara Capponi, Dimitra Chalkia, Timothy A Chan, Hakan Doga, Frederik F. Flother, Gad Getz, Mark Goldsmith, Tanvi Gujarati, Aldo Guzman-Saenz, Dimitrios Iliopoulos, Gavin O. Jones, Stefan Knecht, Dhiraj Madan, Sabrina Maniscalco, Nicola Mariella, Joseph A. Morrone, Khadijeh Najafi, Pushpak Pati, Daniel Platt, Maria Anna Rapsomaniki, Anupama Ray, Kahn Rhrissorrakrai, Omar Shehab, Ivano Tavernelli, Meltem Tolunay, Filippo Utro, Stefan Woerner, Sergiy Zhuk, Jeannette M. Garcia, Laxmi Parida

In recent years, there has been tremendous progress in the development of quantum computing hardware, algorithms and services leading to the expectation that in the near future quantum computers will be capable of performing simulations for natural science applications, operations research, and machine learning at scales mostly inaccessible to classical computers. Whereas the impact of quantum computing has already started to be recognized in fields such as cryptanalysis, natural science simulations, and optimization among others, very little is known about the full potential of quantum computing simulations and machine learning in the realm of healthcare and life science (HCLS). Herein, we discuss the transformational changes we expect from the use of quantum computation for HCLS research, more specifically in the field of cell-centric therapeutics. Moreover, we identify and elaborate open problems in cell engineering, tissue modeling, perturbation modeling, and bio-topology while discussing candidate quantum algorithms for research on these topics and their potential advantages over classical computational approaches.

Comments: 6 figures

Subjects: **Quantum Physics (quant-ph)**; Quantitative Methods (q-bio.QM)

Cite as: arXiv:2307.05734 **[quant-ph]**

(or arXiv:2307.05734v2 **[quant-ph]** for this version)

https://doi.org/10.48550/arXiv.2307.05734

Submission history

From: Kahn Rhrissorrakrai [view email]

[v1] Tue, 11 Jul 2023 19:02:37 UTC (22,487 KB)

[v2] Tue, 1 Aug 2023 14:44:38 UTC (22,490 KB)

Quantum computing for clinical trial design and optimization

arXiv > quant-ph > arXiv:2404.13113

Search...

Help | Advan

Quantum Physics

[Submitted on 19 Apr 2024]

Towards quantum computing for clinical trial design and optimization: A perspective on new opportunities and challenges

Hakan Doga, M. Emre Sahin, Joao Bettencourt-Silva, Anh Pham, Eunyoung Kim, Alan Andress, Sudhir Saxena, Aritra Bose, Laxmi Parida, Jan Lukas Robertus, Hideaki Kawaguchi, Radwa Soliman, Daniel Blankenberg

Clinical trials are pivotal in the drug discovery process to determine the safety and efficacy of a drug candidate. The high failure rates of these trials are attributed to deficiencies in clinical model development and protocol design. Improvements in the clinical drug design process could therefore yield significant benefits for all stakeholders involved. This paper examines the current challenges faced in clinical trial design and optimization, reviews established classical computational approaches, and introduces quantum algorithms aimed at enhancing these processes. Specifically, the focus is on three critical aspects: clinical trial simulations, site selection, and cohort identification. This study aims to provide a comprehensive framework that leverages quantum computing to innovate and refine the efficiency and effectiveness of clinical trials.

Subjects: **Quantum Physics (quant-ph)**; Emerging Technologies (cs.ET)

Cite as: arXiv:2404.13113 **[quant-ph]**

(or arXiv:2404.13113v1 **[quant-ph]** for this version)

https://doi.org/10.48550/arXiv.2404.13113

Submission history

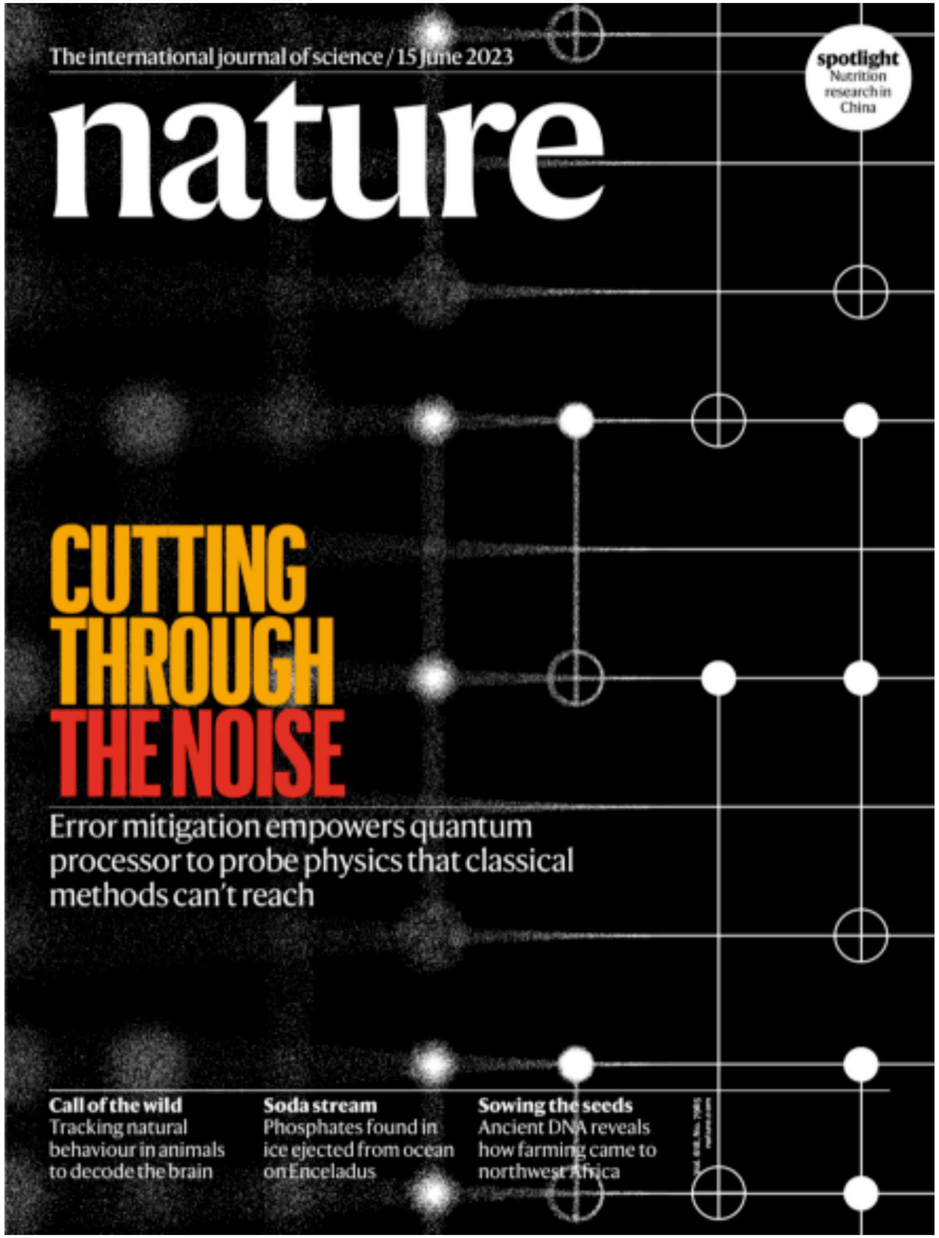
From: Hakan Doga [view email]

[v1] Fri, 19 Apr 2024 18:00:25 UTC (2,720 KB)

Quantum computing for sustainability

white paper coming up soon in arXiv

sustainability



Article

Evidence for the utility of quantum computing before fault tolerance

https://doi.org/10.1038/s41586-023-06096-3

Received: 24 February 2023

Accepted: 18 April 2023

Published online: 14 June 2023

Open access

Check for updates

Youngseok Kim[1,6]✉, Andrew Eddins[2,6]✉, Sajant Anand[3], Ken Xuan Wei[1], Ewout van den Berg[1], Sami Rosenblatt[1], Hasan Nayfeh[1], Yantao Wu[3,4], Michael Zaletel[3,5], Kristan Temme[1] & Abhinav Kandala[1]✉

Quantum computing promises to offer substantial speed-ups over its classical counterpart for certain problems. However, the greatest impediment to realizing its full potential is noise that is inherent to these systems. The widely accepted solution to this challenge is the implementation of fault-tolerant quantum circuits, which is out of reach for current processors. Here we report experiments on a noisy 127-qubit processor and demonstrate the measurement of accurate expectation values for circuit volumes at a scale beyond brute-force classical computation. We argue that this represents evidence for the utility of quantum computing in a pre-fault-tolerant era. These experimental results are enabled by advances in the coherence and calibration of a superconducting processor at this scale and the ability to characterize[1] and controllably manipulate noise across such a large device. We establish the accuracy of the measured expectation values by comparing them with the output of exactly verifiable circuits. In the regime of strong entanglement, the quantum computer provides correct results for which leading classical approximations such as pure-state-based 1D (matrix product states, MPS) and 2D (isometric tensor network states, isoTNS) tensor network methods[2,3] break down. These experiments demonstrate a foundational tool for the realization of near-term quantum applications[4,5].

Quantum dynamics using 127 qubits in 2D

- **Dynamics in a transverse-field Ising model**
- **Time steps up to *n*=20**
- **Hard to simulate it using classical computers!?**

Summary & Conclusion

- 100量子ビット以上を有する量子コンピュータ実機が利用できるようになり、100量子ビット以上を用いた"量子計算"が報告され始めた（→ Era of **Quantum Utility**）
- 平均利用量子ビット数は10~20量子ビット程度と規模が小さい（← "**Quantum Advantage**"には50量子ビット程度以上の量子計算が必要、2031年には到達?）
- 量子化学計算への応用などは、特に規模が小さい（← VQEなどは、量子回路構築、変分パラメータ最適化可能性も含めたscalability、観測・error mitigationによるoverheadなど課題多い）
- 従来の量子-古典ハイブリッドパラダイムを超えたHPCと量子コンピュータの連携が必要：
  Quantum-Centric Supercomputing, 量子スーパーコンピューティング, …
- Early-FTQCあるいはFTQCを見据えたアプリケーション開発
- HPCを用いた100量子ビット以上の量子計算シミュレーション開発