Variational quantum simulations on noisy quantum devices: strategies for circuit design and error mitigation

Stefan Kühn

The Cyprus Institute
RESEARCH • TECHNOLOGY • INNOVATION

CaSToRC

Humboldt Kolleg Kitzbühel
2022/07/01

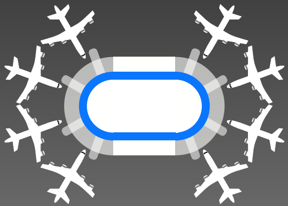
Motivation

Quantum computers have the potential to drive (scientific) innovation

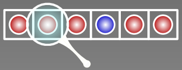
- Factoring

$$70747 = 263 \times 269$$

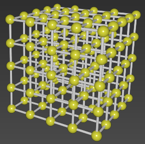
- Optimization



- Searching databases



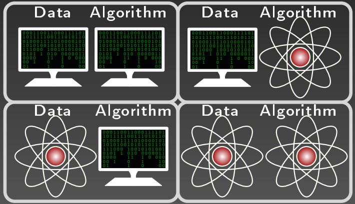
- Quantum systems
  - Lattice field theory



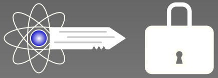
  - Quantum chemistry

  - Material science
  - ...

- Machine learning



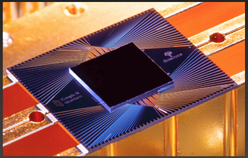
- Cryptography



- ...

Motivation

On the verge of the NISQ era



- NISQ devices with $\mathcal{O}(100)$ qubits are available
- Noise significantly limits the applicability
  - No quantum error correction

J. Preskill, Quantum 2, 79 (2018)

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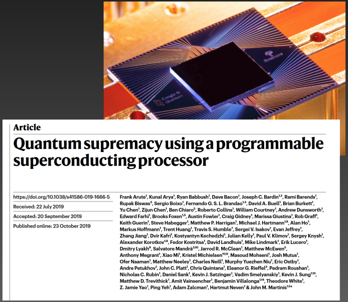

Article

Quantum supremacy using a programmable superconducting processor

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Frank Arute[1], Kunal Arya[1], Ryan Babbush[1], Dave Bacon[1], Joseph C. Bardin[1,2], Rami Barends[1], Rupak Biswas[3], Sergio Boixo[1], Fernando G. S. L. Brandao[1,4], David A. Buell[1], Brian Burkett[1], Yu Chen[1], Zijun Chen[1], Ben Chiaro[5], Roberto Collins[1], William Courtney[1], Andrew Dunsworth[1], Edward Farhi[1], Brooks Foxen[1,5], Austin Fowler[1], Craig Gidney[1], Marissa Giustina[1], Rob Graff[1], Keith Guerin[1], Steve Habegger[1], Matthew P. Harrigan[1], Michael J. Hartmann[1,6], Alan Ho[1], Markus Hoffmann[1], Trent Huang[1], Travis S. Humble[7], Sergei V. Isakov[1], Evan Jeffrey[1], Zhang Jiang[1], Dvir Kafri[1], Kostyantyn Kechedzhi[1], Julian Kelly[1], Paul V. Klimov[1], Sergey Knysh[1], Alexander Korotkov[1,8], Fedor Kostritsa[1], David Landhuis[1], Mike Lindmark[1], Erik Lucero[1], Dmitry Lyakh[9], Salvatore Mandrà[3,10], Jarrod R. McClean[1], Matthew McEwen[5], Anthony Megrant[1], Xiao Mi[1], Kristel Michielsen[11,12], Masoud Mohseni[1], Josh Mutus[1], Ofer Naaman[1], Matthew Neeley[1], Charles Neill[1], Murphy Yuezhen Niu[1], Eric Ostby[1], Andre Petukhov[1], John C. Platt[1], Chris Quintana[1], Eleanor G. Rieffel[3], Pedram Roushan[1], Nicholas C. Rubin[1], Daniel Sank[1], Kevin J. Satzinger[1], Vadim Smelyanskiy[1], Kevin J. Sung[1,13], Matthew D. Trevithick[1], Amit Vainsencher[1], Benjamin Villalonga[1,14], Theodore White[1], Z. Jamie Yao[1], Ping Yeh[1], Adam Zalcman[1], Hartmut Neven[1] & John M. Martinis[1,5]*

J. Preskill, Quantum 2, 79 (2018)
F. Arute et al., Nature 574, 5050 (2019)

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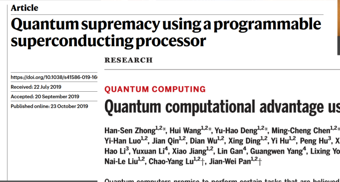

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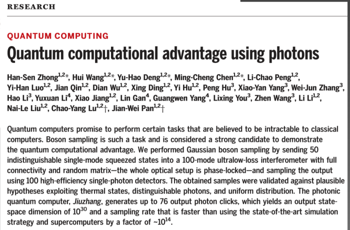

RESEARCH

QUANTUM COMPUTING

Quantum computational advantage using photons

Han-Sen Zhong[1,2]*, Hui Wang[1,2]*, Yu-Hao Deng[1,2]*, Ming-Cheng Chen[1,2]*, Li-Chao Peng[1,2], Yi-Han Luo[1,2], Jian Qin[1,2], Dian Wu[1,2], Xing Ding[1,2], Yi Hu[1,2], Peng Hu[3], Xiao-Yan Yang[3], Wei-Jun Zhang[3], Hao Li[3], Yuxuan Li[4], Xiao Jiang[1,2], Lin Gan[4], Guangwen Yang[4], Lixing You[3], Zhen Wang[3], Li Li[1,2], Nai-Le Liu[1,2], Chao-Yang Lu[1,2]†, Jian-Wei Pan[1,2]†

Quantum computers promise to perform certain tasks that are believed to be intractable to classical computers. Boson sampling is such a task and is considered a strong candidate to demonstrate the quantum computational advantage. We performed Gaussian boson sampling by sending 50 indistinguishable single-mode squeezed states into a 100-mode ultralow-loss interferometer with full connectivity and random matrix—the whole optical setup is phase-locked—and sampling the output using 100 high-efficiency single-photon detectors. The obtained samples were validated against plausible hypotheses exploiting thermal states, distinguishable photons, and uniform distribution. The photonic quantum computer, *Jiuzhang*, generates up to 76 output photon clicks, which yields an output state-space dimension of 10^{30} and a sampling rate that is faster than using the state-of-the-art simulation strategy and supercomputers by a factor of ~10^{14}.

F. Arute et al., Nature 574, 5050 (2019)
H.-S. Zhong et al., Science 370, 1460 (2020)

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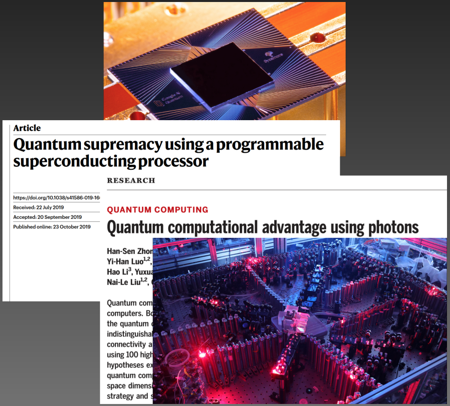

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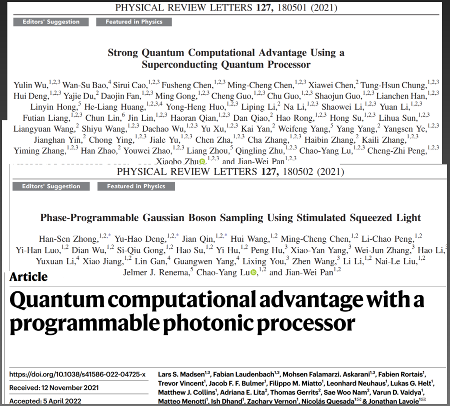

PHYSICAL REVIEW LETTERS **127,** 180501 (2021)

Editors' Suggestion | Featured in Physics

Strong Quantum Computational Advantage Using a Superconducting Quantum Processor

Yulin Wu,[1,2,3] Wan-Su Bao,[4] 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,[5] He-Liang Huang,[1,2,3,4] 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] Yu Xu,[1,2,3] Kai Yan,[2] Weifeng Yang,[5] 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,[5] Qingling Zhu,[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]

PHYSICAL REVIEW LETTERS **127,** 180502 (2021)

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Phase-Programmable Gaussian Boson Sampling Using Stimulated Squeezed Light

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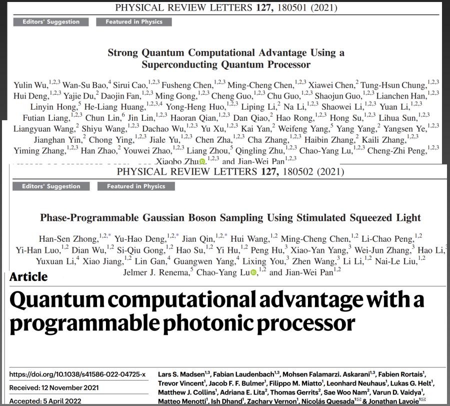
F. Arute et al., Nature 574, 5050 (2019)
H.-S. Zhong et al., Science 370, 1460 (2020)
Y. Wu et al., PRL 127, 180501 (2021), Han-Sen Zhong et al., PRL 127, 180502 (2021), L. S. Madsen et al., Nature 606, 75 (2022)

Motivation

On the verge of the NISQ era

- NISQ devices with $\mathcal{O}(100)$ qubits are available
- Noise significantly limits the applicability
  - No quantum error correction
- Current NISQ devices have already outperformed classical devices
- Large devices expected soon
  - IBM: 1000 qubits by the end of 2023
  - Google: 10^6 error-corrected qubits by 2029



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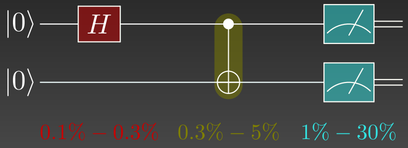
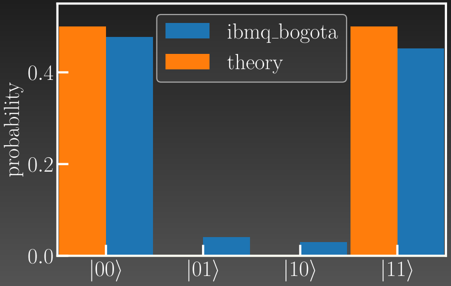
https://research.ibm.com/blog/ibm-quantum-roadmap, https://blog.google/technology/ai/unveiling-our-new-quantum-ai-campus/

Motivation

Running quantum programs





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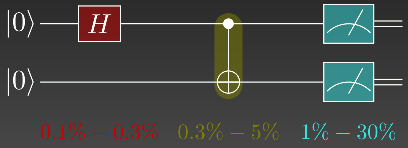

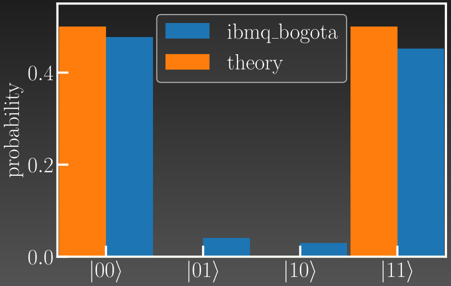

- Errors arise from:
  - Imperfect gates and crosstalk
  - Coupling to environment
  - Measurement/readout

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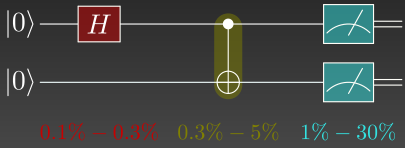

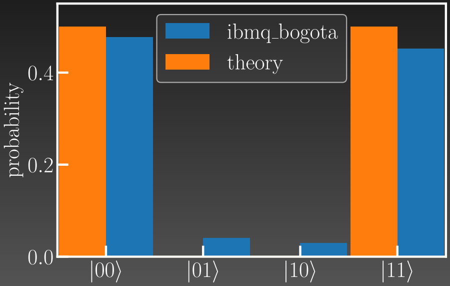

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  - Measurement/readout

NISQ devices do not allow for executing deep circuits faithfully due to noise!

Motivation

Key ingredients that are required to benefit from quantum computers

Algorithms

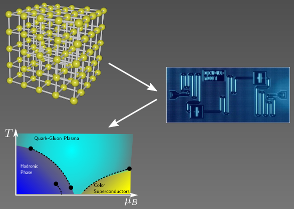
- Mapping problems to a quantum device?
- Resource-efficient implementation?

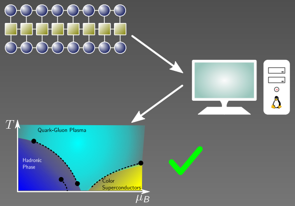
Validation

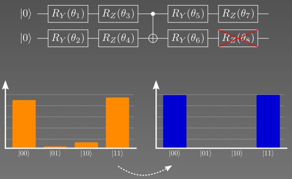
- Classical simulation of quantum programs
- Benchmarking data for unknown regimes

Noise reduction

- Design of optimal parametric circuits?
- Mitigation of effects of noise?







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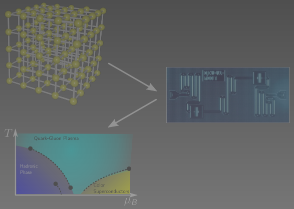

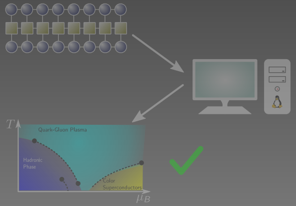

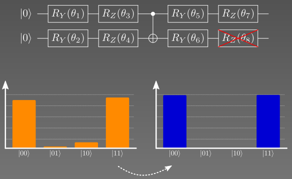

Outline

1. Motivation
2. Variational Quantum Algorithms
3. Dimensional Expressivity Analysis
4. Readout error mitigation
5. Summary and Outlook

1 Motivation

2 Variational Quantum Algorithms

3 Dimensional Expressivity Analysis

4 Readout error mitigation

5 Summary and Outlook

Variational Quantum Algorithms

Variational Quantum Eigensolver

- Hybrid quantum-classical algorithm for finding ground states of Hamiltonians $\mathcal{H}$
- Define the cost function to be minimized

$$\mathcal{C}(\vec{\theta}) = \langle \psi(\vec{\theta}) | \mathcal{H} | \psi(\vec{\theta}) \rangle$$

Peruzzo et al., Nat. Commun. 5, 1 (2014)
J. R. McClean et al., New J. Phys. 18, 023023 (2016)

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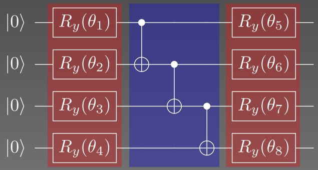
- Realize a parametric ansatz $|\psi(\vec{\theta})\rangle$ by a parametric quantum circuit



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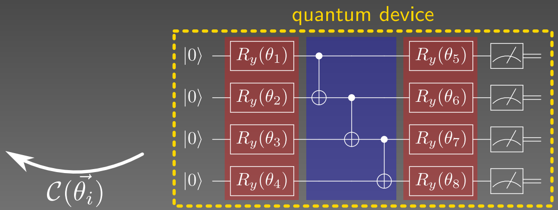
- Measure the cost function $\mathcal{C}(\vec{\theta})$ on the quantum device



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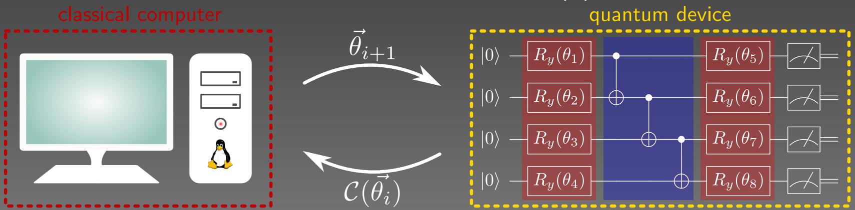
- Realize a parametric ansatz $|\psi(\vec{\theta})\rangle$ by a parametric quantum circuit
- Measure the cost function $\mathcal{C}(\vec{\theta})$ on the quantum device
- Optimize the parameters classically to minimize $\mathcal{C}(\vec{\theta})$



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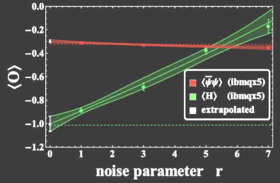
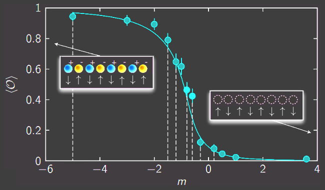
Variational Quantum Algorithms

Examples for applications in particle physics and beyond

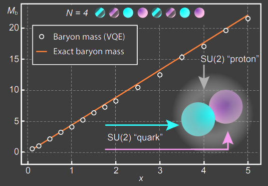
Schwinger model PBC



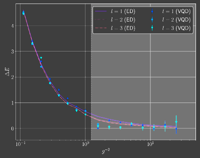
Schwinger model OBC



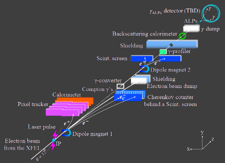
SU(2) gauge model OBC



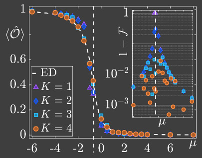
U(1) in (2+1)d



Particle tracking



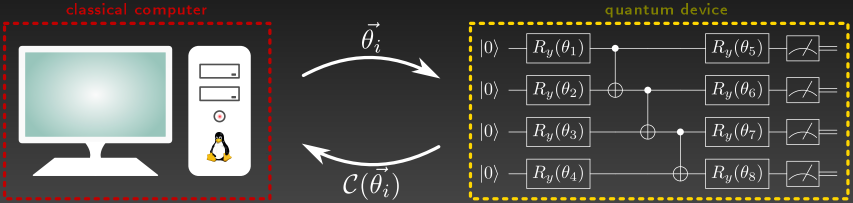
Schwinger model OBC



N. Klco et al., Phys. Rev. A 98, 032331 (2018); C. Kokail et al., Nature 569, 355 (2019); Y. Y. Atas et al., Nat. Commun. 12, 6499 (2021)
G. Clemente et al., arXiv:2206.12454; L. Funcke et al., arXiv:2202.06874; R. R. Ferguson et al., PRL 126, 220501 (2021)

Variational Quantum Algorithms

Variational Quantum Algorithms

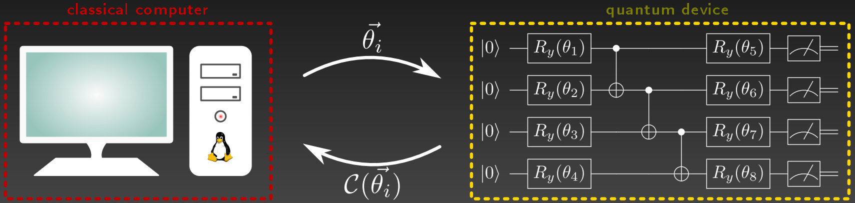


Advantages

- Flexible ansatz design
- Hamiltonian exists only as a measurement
- Partially resilient to systematic errors

Variational Quantum Algorithms

Variational Quantum Algorithms



Advantages

- Flexible ansatz design
- Hamiltonian exists only as a measurement
- Partially resilient to systematic errors

Challenges

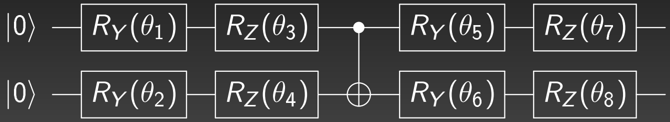
- How to choose an expressive ansatz?
- How to avoid redundant parameters?
- How to deal with effects of noise?

1 Motivation
2 Variational Quantum Algorithms
3 Dimensional Expressivity Analysis
4 Readout error mitigation
5 Summary and Outlook

Dimensional Expressivity Analysis

Dimensional Expressivity Analysis

- **Goal:** given a parametric quantum circuit, remove redundant parameters



- **Method:** geometrical approach, circuit as a map that maps the input parameters to the state space of the quantum device

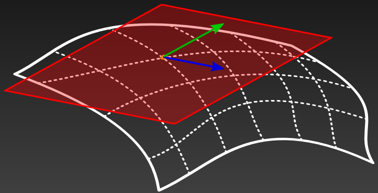
$$C : \vec{\theta} \mapsto |C(\vec{\theta})\rangle = R_Z(\theta_8) \dots R_Y(\theta_1) \, |0\rangle \otimes |0\rangle$$

- Parameter space P: real manifold
- Image of C: **circuit manifold** $\mathcal{M}$
- Which parameters are necessary to generate the circuit manifold $\mathcal{M}$?

Lena Funcke, Tobias Hartung, Karl Jansen, SK, Paolo Stornati, Quantum 5, 422 (2021)

Dimensional Expressivity Analysis

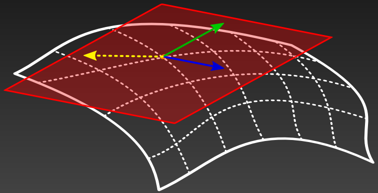
- The tangent space of $\mathcal{M}$ is spanned by the tangent vectors $|\partial_j C(\vec{\theta})\rangle$



Dimensional Expressivity Analysis

Dimensional Expressivity Analysis

- The tangent space of $\mathcal{M}$ is spanned by the tangent vectors $|\partial_j C(\vec{\theta})\rangle$
- θ_k is redundant iff $|\partial_k C(\vec{\theta})\rangle$ is a linear combination of $|\partial_j C(\vec{\theta})\rangle$, $j \neq k$



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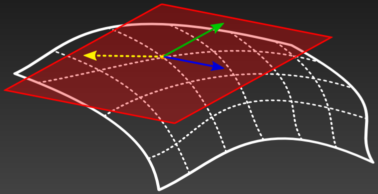

Algorithm

- θ_1 is never redundant as long as the corresponding parametric gate is nontrivial
- Check whether $|\partial_{k+1} C(\vec{\theta})\rangle$ is a linear combination of $|\partial_1 C(\vec{\theta})\rangle, \ldots, |\partial_k C(\vec{\theta})\rangle$
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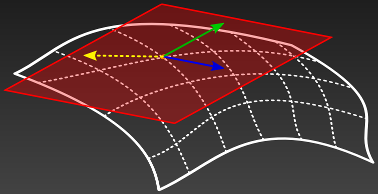

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- Check whether $|\partial_{k+1} C(\vec{\theta})\rangle$ is a linear combination of $|\partial_1 C(\vec{\theta})\rangle, \ldots, |\partial_k C(\vec{\theta})\rangle$
- Remove redundant parameters
  - Parameter removal implies setting the parameter to a constant value
  - Rotation gates (e.g. $\exp(-\frac{i}{2}\vartheta X)$): choose the parameter $\vartheta = 0$ to achieve an $\mathbb{1}$

Lena Funcke, Tobias Hartung, Karl Jansen, SK, Paolo Stornati, Quantum 5, 422 (2021)

Dimensional Expressivity Analysis

Checking for parameter independence

- θ_1 is never redundant as long as corresponding parametric gate is nontrivial
- For θ_k, $k = 2, ..., n$ we can check the rank of the (real) Jacobian

$$J_k = \begin{pmatrix} | & & | \\ \Re|\partial_1 C\rangle & \dots & \Re|\partial_k C\rangle \\ | & & | \\ | & & | \\ \Im|\partial_1 C\rangle & \dots & \Im|\partial_k C\rangle \\ | & & | \end{pmatrix}$$

$\Rightarrow$ If the matrix J_k has full rank then θ_k is independent

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$\Rightarrow$ If the matrix J_k has full rank then θ_k is independent

- Instead of checking the rank of J_k one can also compute the rank of $S_k = J_k^T J_k$

Tangent vectors require an exponential amount of memory!

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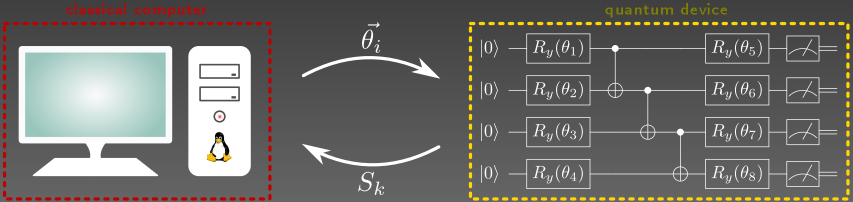
Dimensional Expressivity Analysis

Can we use a hybrid-quantum classical approach for the Dimensonal Expressivity Analysis?



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Dimensional Expressivity Analysis

Hybrid Quantum-Classical Dimensional Expressivity Analysis

- Since the first parameter is always nontrivial $S_1 = \frac{1}{4}$
- For $k \geq 2$ the $k \times k$ matrices $S_k = J_k^T J_k$ can be cast into the form

$$S_k = \begin{pmatrix} S_{k-1} & A_k \\ A_k^T & \frac{1}{4} \end{pmatrix} \qquad \text{with} \qquad A_k = \begin{pmatrix} \Re \left\langle \partial_1 C(\vec{\theta}) \middle| \partial_k C(\vec{\theta}) \right\rangle \\ \vdots \\ \Re \left\langle \partial_{k-1} C(\vec{\theta}) \middle| \partial_k C(\vec{\theta}) \right\rangle \end{pmatrix}$$

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- For $R_G(\vartheta) = \exp(-\frac{i}{2}\vartheta G)$ where G is a gate, the derivative is essentially a circuit

$$|R_G\rangle = |0\rangle \;-\!\boxed{R_G(\vartheta)}\!- \qquad \Rightarrow \qquad 2i\,|\partial_\theta R_G\rangle = |0\rangle \;-\!\boxed{R_G(\vartheta)}\!-\!\boxed{G}\!-$$

- Up to an imaginary factor $|\partial_j C(\vec{\theta})\rangle$ can be prepared on a quantum device

Lena Funcke, Tobias Hartung, Karl Jansen, SK, Paolo Stornati, Quantum 5, 422 (2021)

Dimensional Expressivity Analysis

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- If we can efficiently obtain $\Re\langle\partial_j C(\vec{\theta})|\partial_k C(\vec{\theta})\rangle$ on the quantum device, we can carry out dimensional expressivity analysis efficiently

S. Lloyd, M. Mohseni, P. Rebentrost, arXiv:1307.0411 (2013)
L. Zhao, Z. Zhao, P. Rebentrost, J. Fitzsimons, arXiv:1902.10394 (2019)
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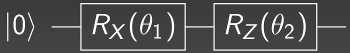

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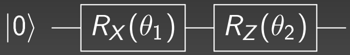
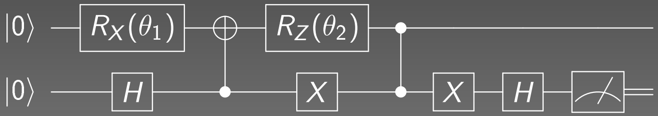


- Circuit for obtaining $\Re\langle\partial_1 C(\vec{\theta})|\partial_2 C(\vec{\theta})\rangle$



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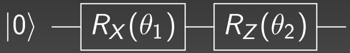

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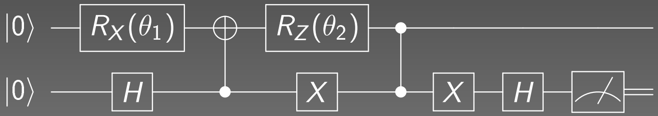

- Real part of the overlap is proportional to the probability for the ancilla being in $|0\rangle$

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Dimensional Expressivity Analysis

Results for a single qubit on quantum hardware

- Simple example circuit

$$|\psi(\theta_4, \theta_3, \theta_2, \theta_1)\rangle = |0\rangle \; - \boxed{R_Z(\theta_1)} - \boxed{R_X(\theta_2)} - \boxed{R_Z(\theta_3)} - \boxed{R_Y(\theta_4)} -$$

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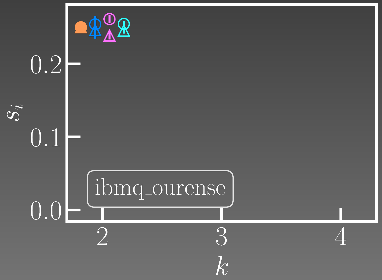
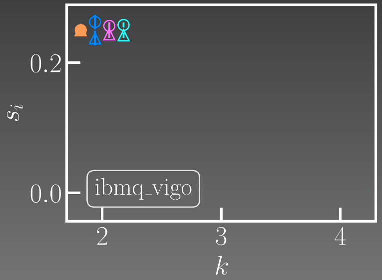
- Results on IBM quantum hardware: spectrum of S_k, $k \geq 2$





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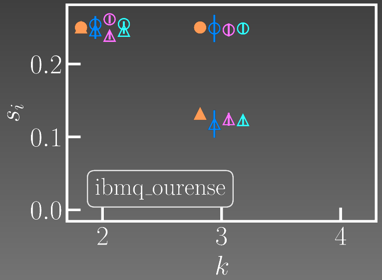

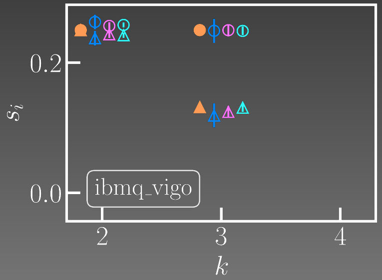

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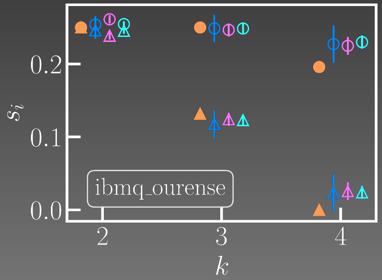

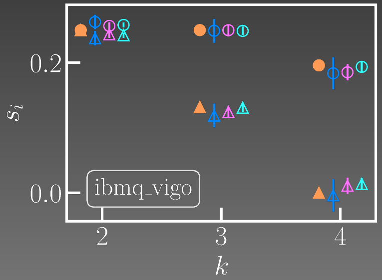

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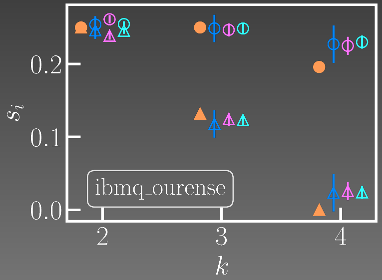

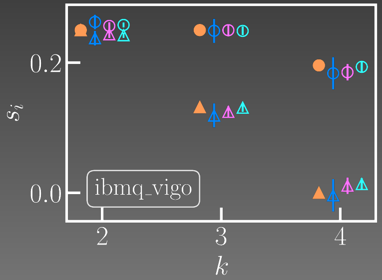

$\Rightarrow$ Number of independent parameters: 3, last gate $R_Y(\theta_4)$ is redundant

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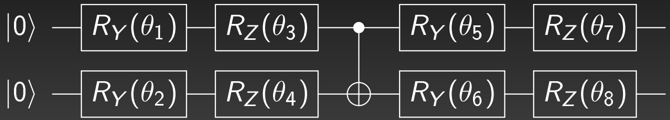
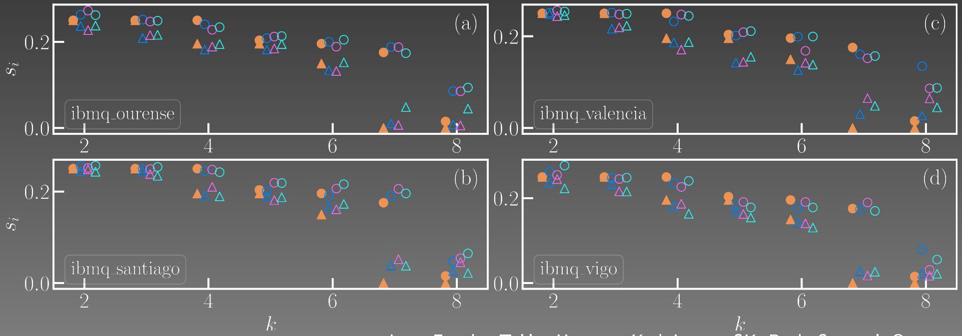
Dimensional Expressivity Analysis

Results for two qubits on quantum hardware

- Circuit we examine





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4.

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Noise mitigation and optimal circuit design

Measurement Error Mitigation

- Goal: **low-overhead**, **resource-efficient** method suitable for current devices

L. Funcke, T. Hartung, K. Jansen, SK, P. Stornati, X. Wang, Phys. Rev. A **105**, 062404 (2022)

Noise mitigation and optimal circuit design

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Readout	Bit Flips	Probability	Effective operator
correct	$0 \to 0,\ 1 \to 1$	$(1-p_0)(1-p_1)$	$\tilde{Z} = Z$
incorrect	$0 \to 1,\ 1 \to 0$	$p_0 p_1$	$\tilde{Z} = -Z$
0 outcome incorrect	$0 \to 1,\ 1 \to 1$	$p_0(1-p_1)$	$\tilde{Z} = -\mathbb{1}$
1 outcome incorrect	$0 \to 0,\ 1 \to 0$	$(1-p_0)p_1$	$\tilde{Z} = \mathbb{1}$

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- Expected value of the noisy operator

$$\mathbb{E}\tilde{Z} = (1-p_0)(1-p_1)Z - p_0 p_1 Z - p_0(1-p_1)\mathbb{1} + (1-p_0)p_1\mathbb{1}$$
$$= (1-p_0-p_1)Z + (p_1-p_0)\mathbb{1}$$

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incorrect	$0 \to 1$, $1 \to 0$	$p_0 p_1$	$\tilde{Z} = -Z$
0 outcome incorrect	$0 \to 1$, $1 \to 1$	$p_0(1-p_1)$	$\tilde{Z} = -\mathbb{1}$
1 outcome incorrect	$0 \to 0$, $1 \to 0$	$(1-p_0)p_1$	$\tilde{Z} = \mathbb{1}$

available from calibration on noisy quantum device

$$\langle\psi| Z |\psi\rangle = \frac{1}{1-p_0-p_1} \times \mathbb{E}\langle\psi| \tilde{Z} |\psi\rangle - \frac{p_0-p_1}{1-p_0-p_1}$$

true expectation value

measurement on noisy quantum device

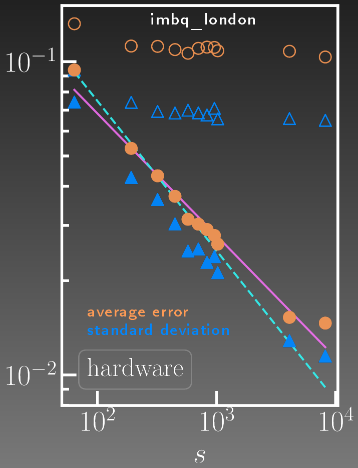
L. Funcke, T. Hartung, K. Jansen, SK, P. Stornati, X. Wang, Phys. Rev. A 105, 062404 (2022)

Noise mitigation and optimal circuit design

Demonstration for two qubits on quantum hardware

- Results for **IBM quantum hardware**
- Measure the expectation value of $Z \otimes Z$ for 1050 random parameter sets
- Compute the average and standard deviation of the error

$$\left|\langle\psi|Z \otimes Z|\psi\rangle_{\mathrm{exact}} - \langle\psi|Z \otimes Z|\psi\rangle_{\mathrm{device}}\right|$$



L. Funcke, T. Hartung, K. Jansen, SK, P. Stornati, X. Wang, Phys. Rev. A **105**, 062404 (2022)

Noise mitigation and optimal circuit design

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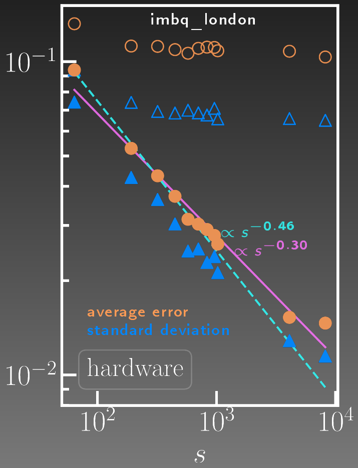
$$|\langle\psi|Z \otimes Z|\psi\rangle_{\text{exact}} - \langle\psi|Z \otimes Z|\psi\rangle_{\text{device}}|$$

$\Rightarrow$ **Improvement** of the error by up to **one order of magnitude**



L. Funcke, T. Hartung, K. Jansen, SK, P. Stornati, X. Wang, Phys. Rev. A **105**, 062404 (2022)

1 Motivation
2 Variational Quantum Algorithms
3 Dimensional Expressivity Analysis
4 Readout error mitigation
5 Summary and Outlook

Summary and Outlook

Dimensional expressivity analysis

- Method for identifying redundant parametric gates in a given ansatz
- Can be carried out efficiently in a hybrid quantum-classical manner
- Allows for incorporating/removing symmetries
- Best approximation error can be quantified

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Dimensional expressivity analysis

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Readout error mitigation

- Simple post-processing allowing for correcting readout errors
- Efficient, only polynomial overhead
- Assumption of uncorrelated qubits can be relaxed, correlations can (to a certain extent) be taken into account
- Can potentially be extended to other sources of error

Thank you for your attention!

Questions?

Lena Funcke
(MIT)

Tobias Hartung
(U. Bath)

Karl Jansen
(DESY)

Paolo Stornati
(ICFO)

Manuel
Schneider
(DESY)

Xiaoyang Wang
(Peking
University)

L. Funcke, T. Hartung, K. Jansen, SK, M. Schneider, P. Stornati, X. Wang Phil. Trans. R. Soc. A. 380: 20210062
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L. Funcke, T. Hartung, K. Jansen, SK, P. Stornati, X. Wang Phys. Rev. A 105, 062404 (2022)

Appendix A: Dimensional Expressivity Analysis

Hybrid quantum-classical Dimensional Expressivity Analysis

- $\Re \left\langle \partial_j C(\vec{\theta}) \middle| \partial_k C(\vec{\theta}) \right\rangle$ can be obtained on the quantum device

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Appendix A: Dimensional Expressivity Analysis

Hybrid quantum-classical Dimensional Expressivity Analysis

- $\Re \left\langle \partial_j C(\vec{\theta}) \middle| \partial_k C(\vec{\theta}) \right\rangle$ can be obtained on the quantum device
- In general $\Re \langle \psi | \phi \rangle$ can be measured using an ancilla qubit provided one can prepare the state

$$|\chi\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle \otimes |\psi\rangle + |1\rangle \otimes |\phi\rangle \right)$$

- Applying a Hadamard gate on the ancilla one finds

$$(H \otimes \mathbb{1}) |\chi\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle \otimes (|\psi\rangle + |\phi\rangle) + |1\rangle \otimes (|\psi\rangle - |\phi\rangle) \right)$$

- Probability of measuring the ancilla in zero

$$p(\text{ancilla} = 0) = \frac{1}{2} \left(1 + \Re \langle \psi | \phi \rangle \right)$$

Lena Funcke, Tobias Hartung, Karl Jansen, SK, Paolo Stornati, Quantum 5, 422 (2021)