Fermilab U.S. DEPARTMENT OF ENERGY Office of Science

Quantum algorithms at the Fermilab Quantum Institute

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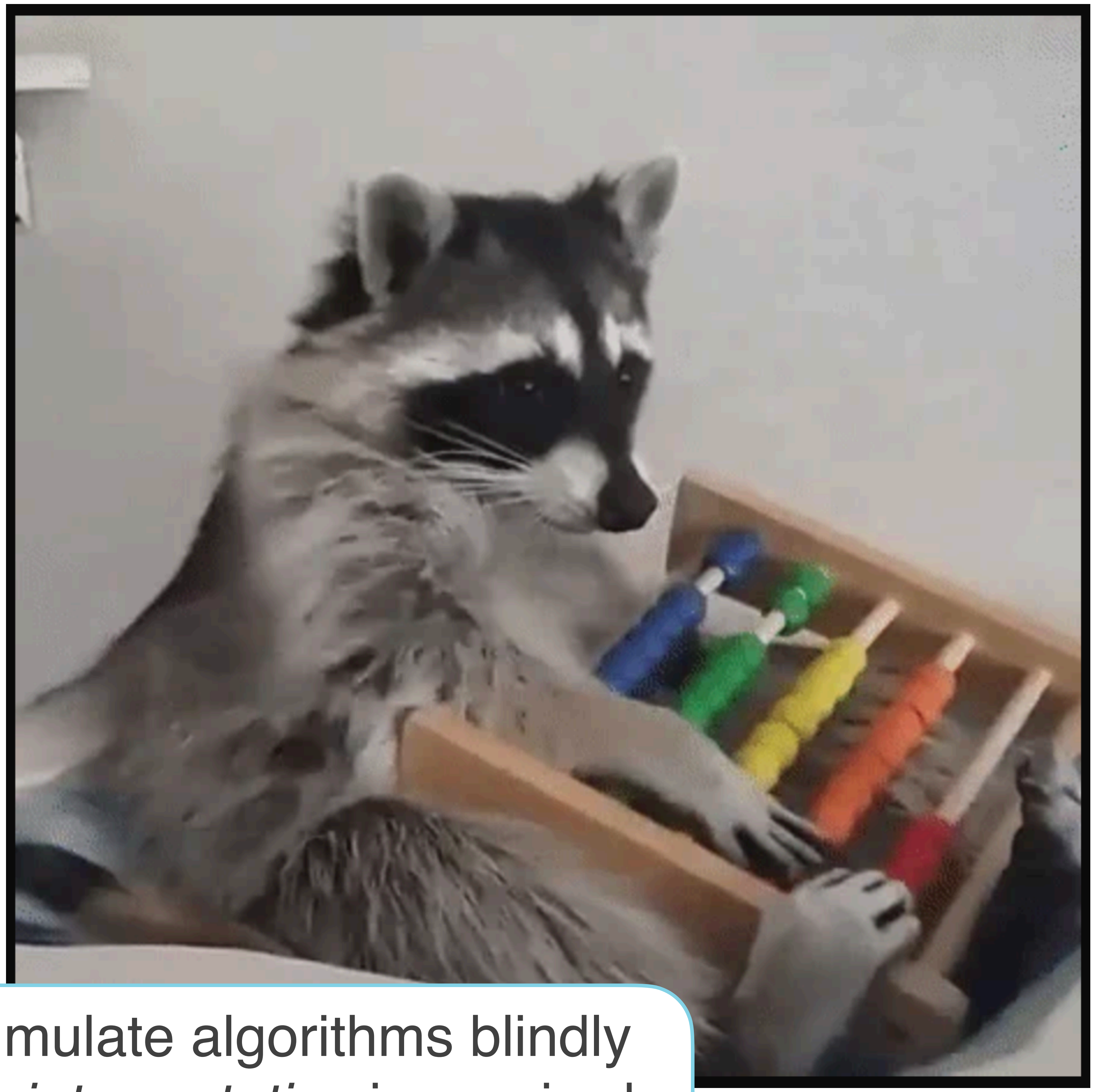
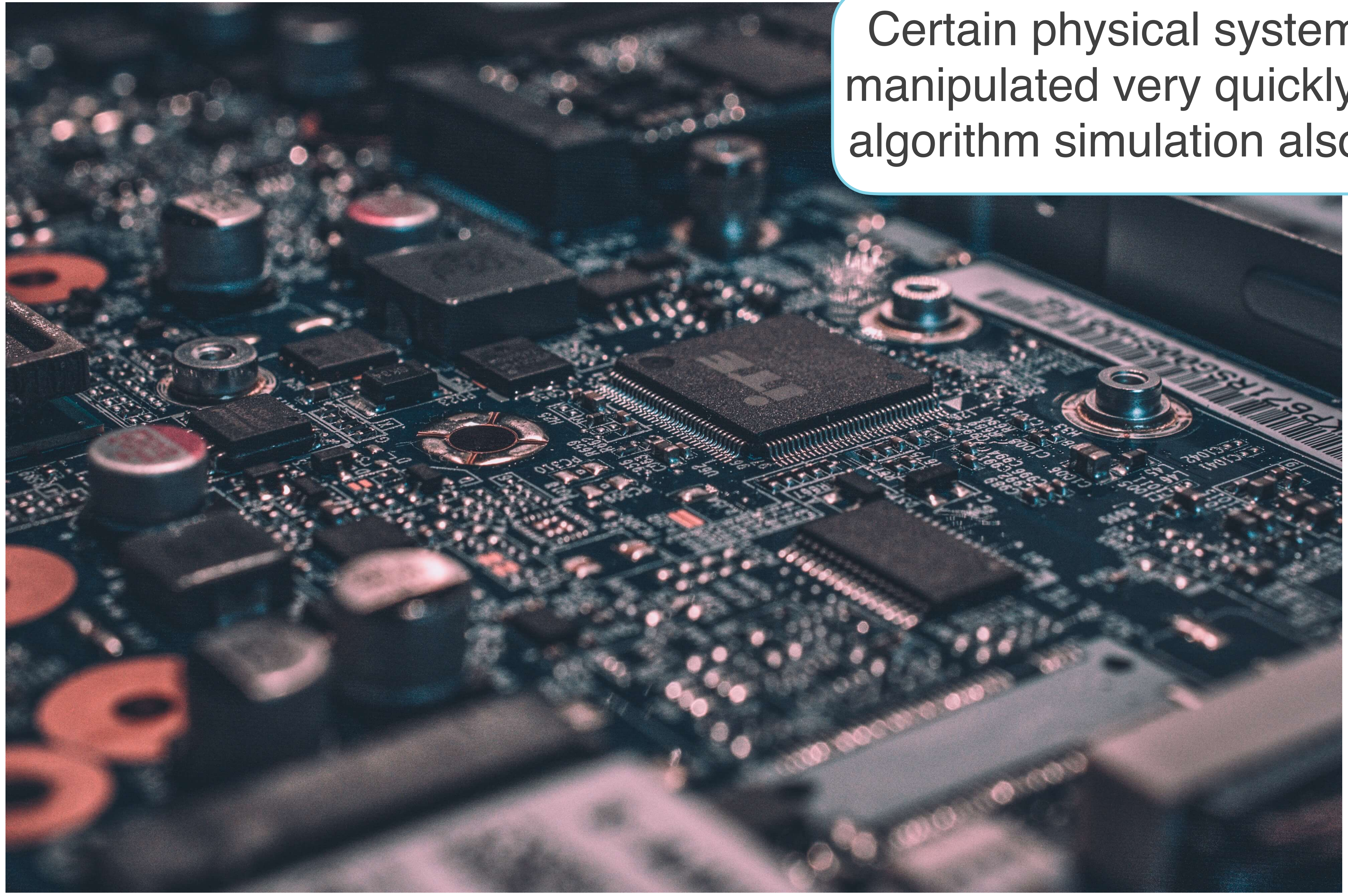
Fermilab User's Meeting, 2022

What is computing?

- First, what is computing? One perspective - it is ***physical simulation of algorithms coupled to interpretation***. We manipulate a physical system according to rules. A metaphysical tower of concepts then allows us to *interpret* the results.

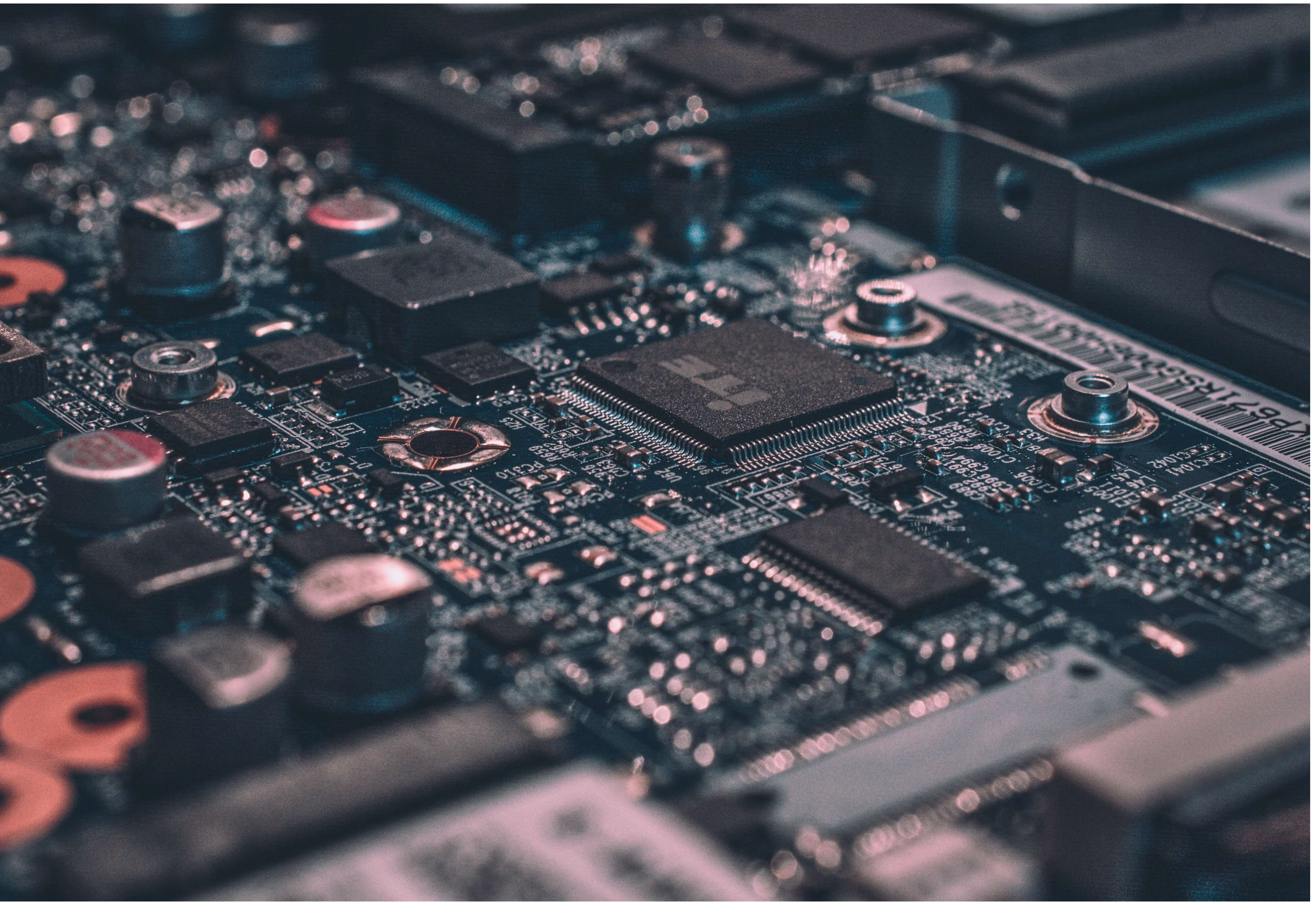


We can simulate algorithms blindly - ultimately *interpretation* is required.



Certain physical systems can be manipulated very quickly - making algorithm simulation also very fast.

What is classical computing?

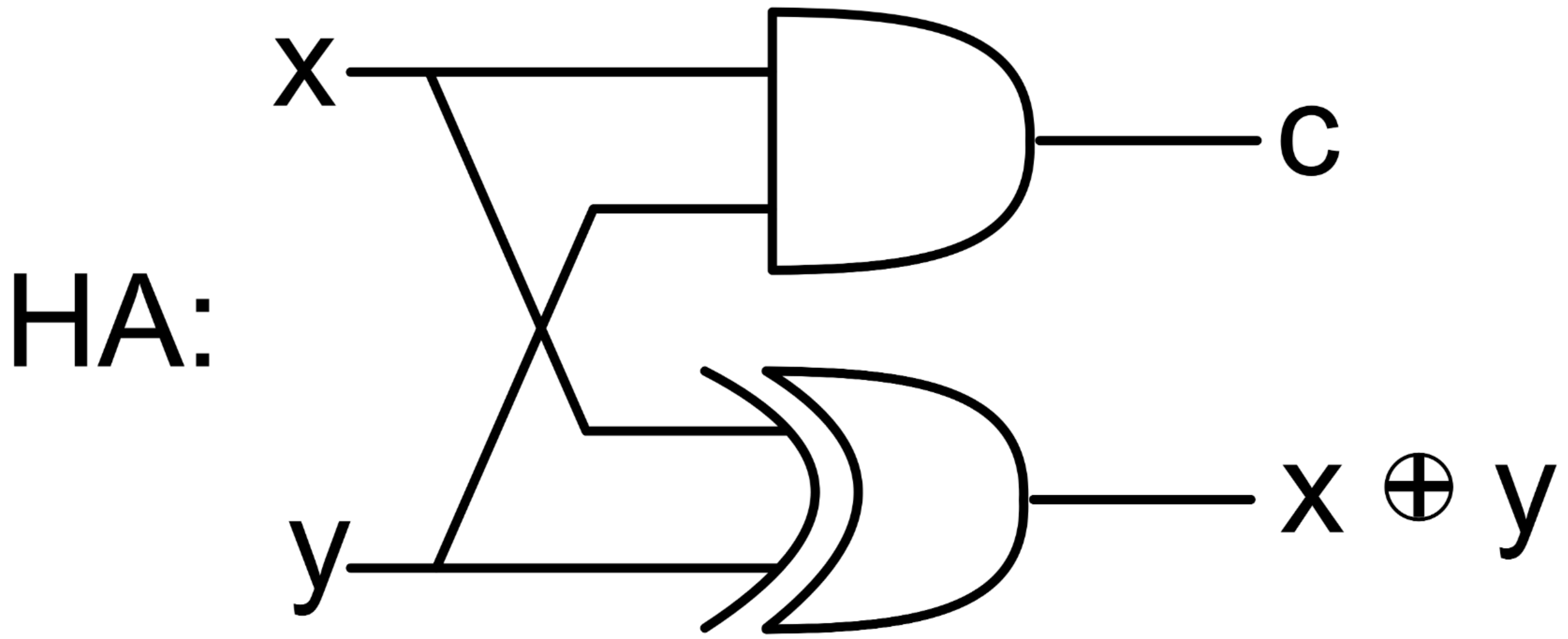


Think about *circuits:*

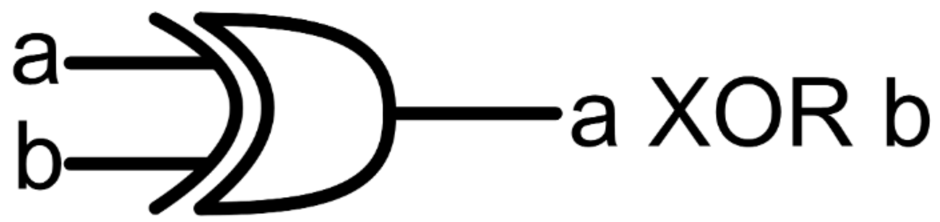
You can see how you would implement a table like this one with logic gates:

```
  0     0     1     1
 +0    +1    +0    +1
---   ---   ---   ---
 00    01    01    10
```

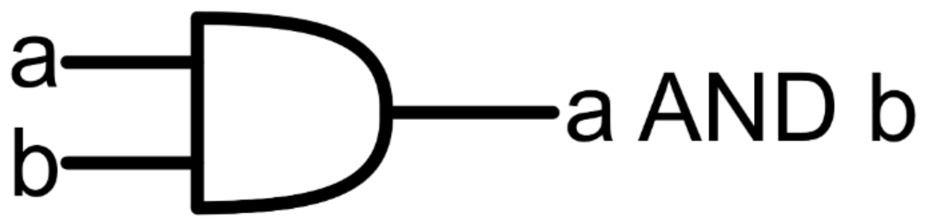
You need two inputs and two outputs. This function is called a *Half Adder*:




```
  0     0     1     1      x
 +0    +1    +0    +1     +y
---   ---   ---   ---   ------
 00    01    01    10   c(x⊕y)
```



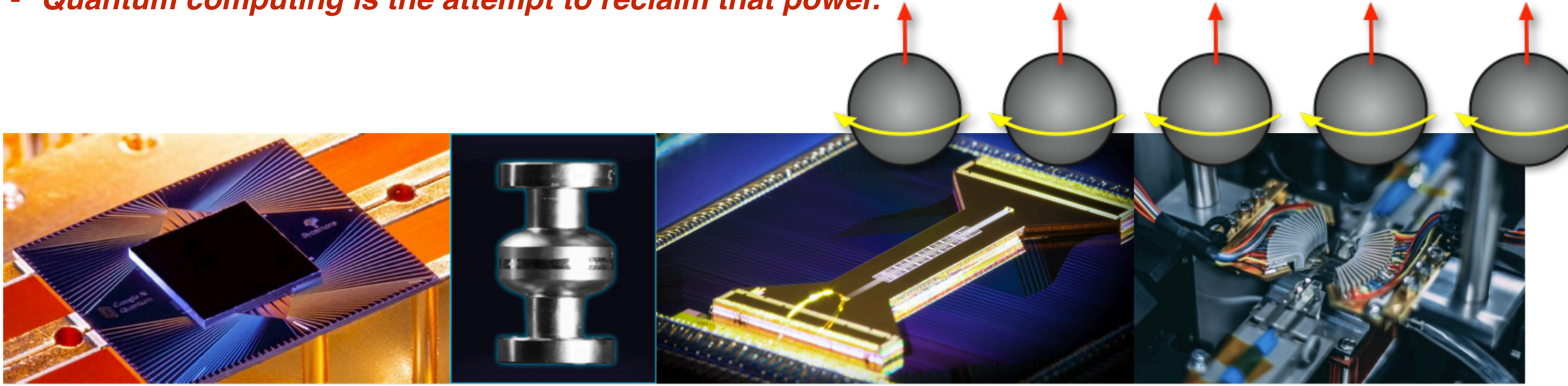
	b = 0	b = 1
a = 0	0	1
a = 1	1	0



	b = 0	b = 1
a = 0	0	0
a = 1	0	1

What is *quantum* computing?

- Draw a contrast to “classical” computing:
  - Nature is quantum mechanical — we may have ***entanglement*** and ***superposition*** of states.
  - ***Measurement*** of a quantum system ***collapses*** the wavefunction, so quantum information is inherently ***fragile.***
  - ***Classical computing gives up any possibility of utilizing entanglement and superposition as part of an algorithm*** in exchange for ***simpler error control protocols***.
  - ***Quantum computing is the attempt to reclaim that power.***



https://ai.googleblog.com/2019/10/quantum-supremacy-using-programmable.html
https://sqms.fnal.gov/research/
https://www.honeywell.com/en-us/company/quantum
https://www.xanadu.ai/hardware

What *is* quantum computing?

https://bit.ly/38bidph

Superposition!

$$|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha \times \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \times \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv \alpha|0\rangle + \beta|1\rangle$$

Tensor products!

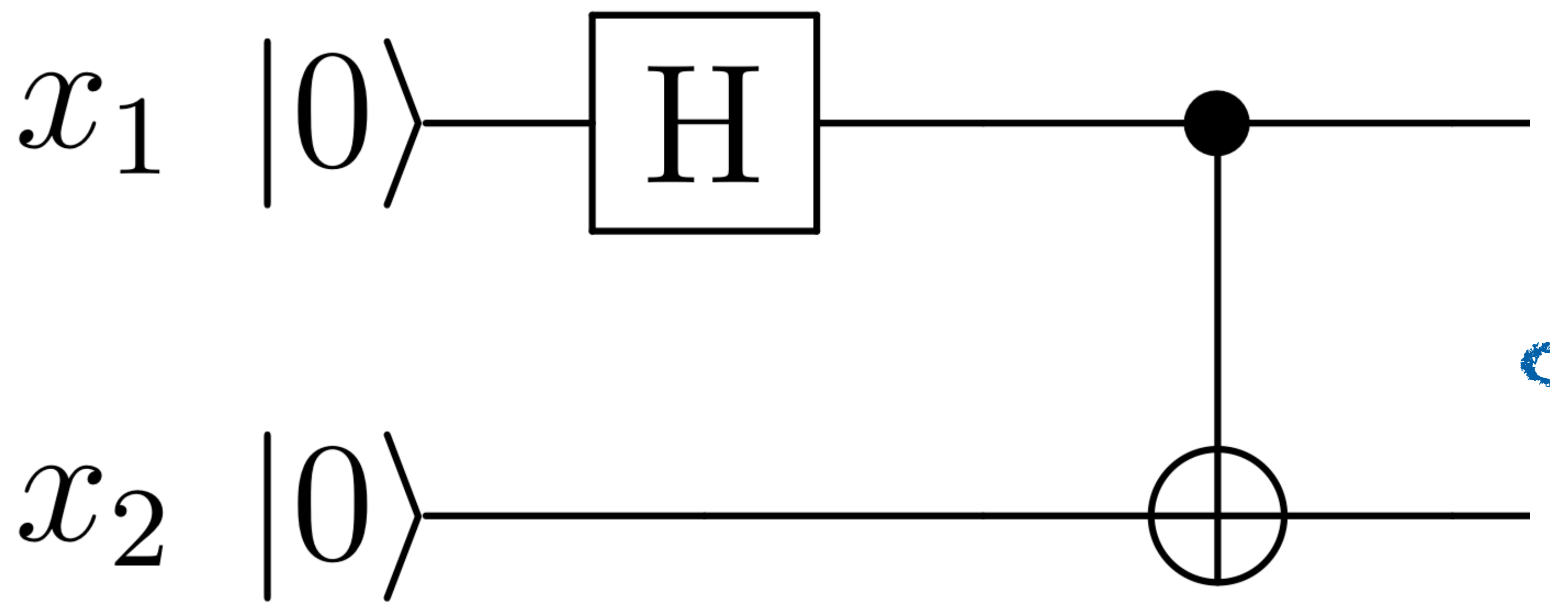
$$|0\rangle|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ 0 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = |00\rangle$$

Unitary operators!

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \equiv |+\rangle$$

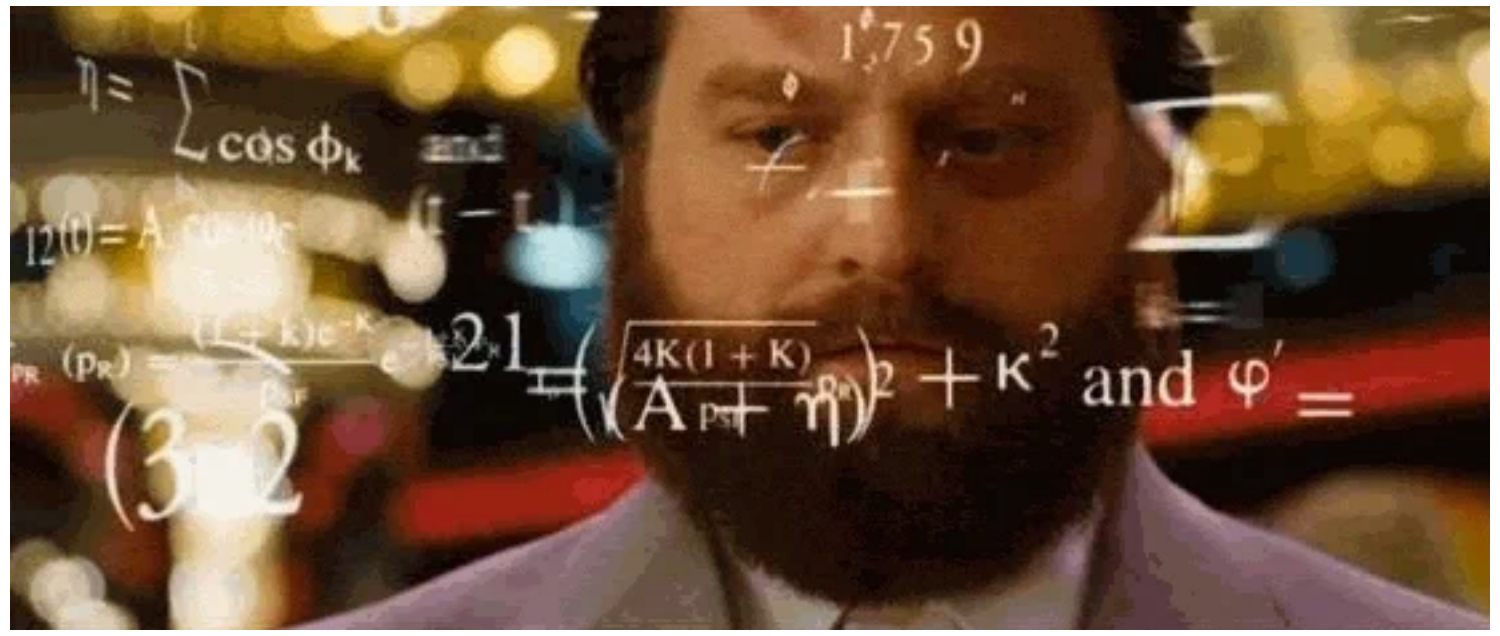
$$H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \equiv |-\rangle$$



Quantum circuits!

Entanglement!

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$



$$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = \frac{1}{\sqrt{2}} \left(\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Bell state - no classical analog!

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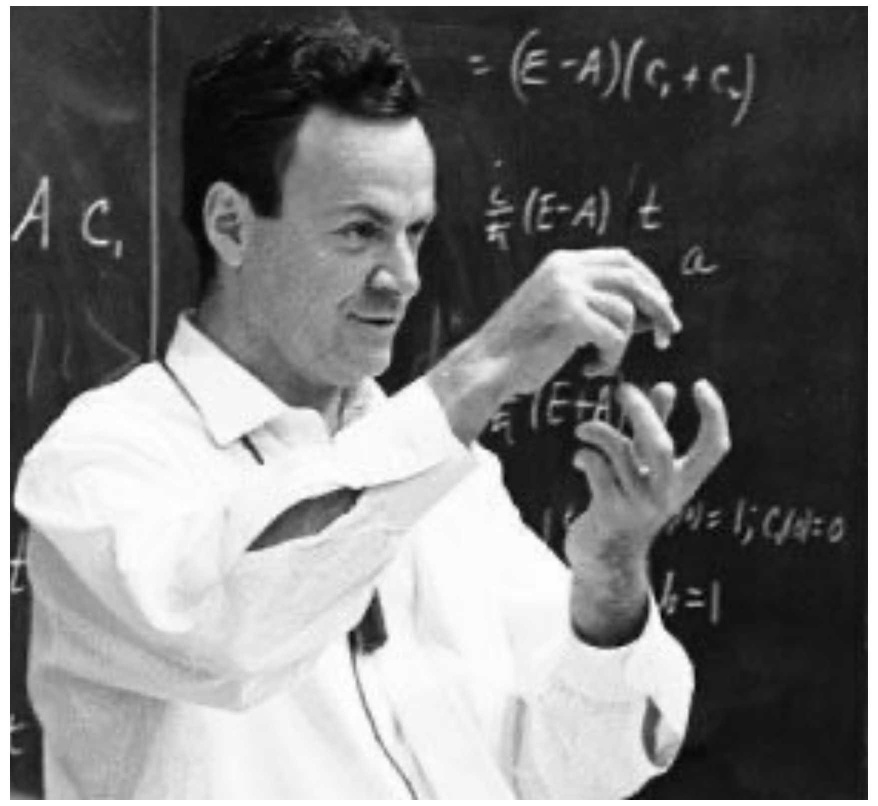
Why is quantum computing interesting for HEP?

- **A quantum computer is a programmable interface to quantum physics experiments.**
  - ***It is a tool for discovery, like a telescope, or a particle accelerator.***
- In HEP we face a set of **computational challenges** in where ***the only practical path to solution requires the utilization of entanglement and superposition as algorithmic primitives.***
- In particular, ***scalable methods for accurately simulating quantum many-body systems are beyond the capabilities of classical computers***.
- Additionally, quantum computers are anticipated to play a ***strong role in future event generators***, speeding up matrix element calculations and even neutrino-nucleus cross section calculations.



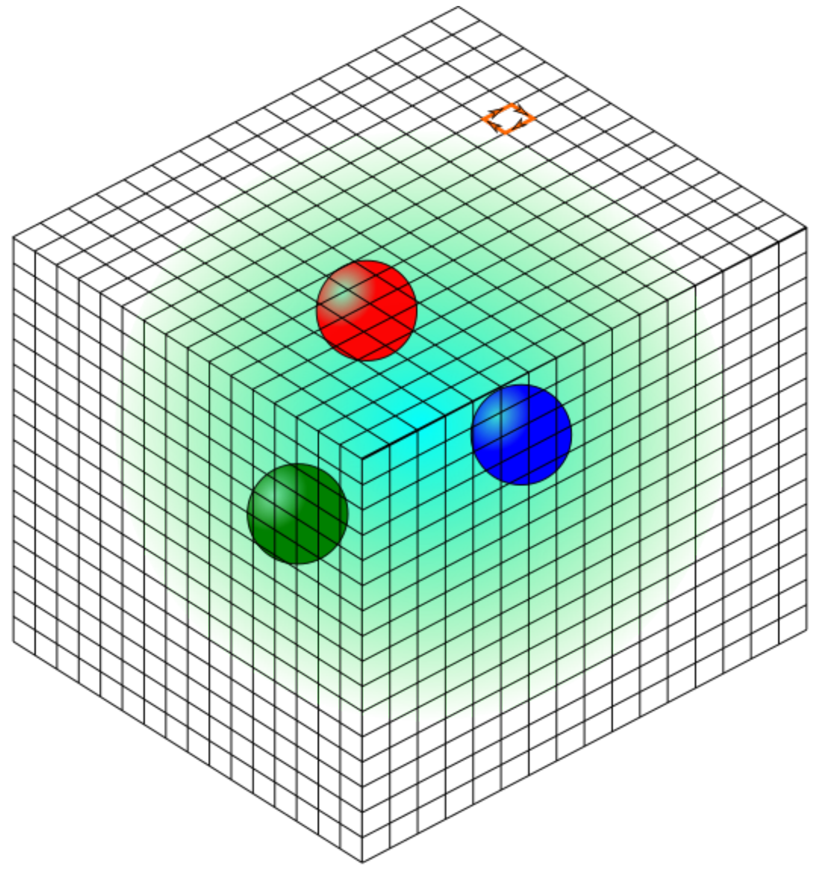


Figure courtesy of H. Lamm

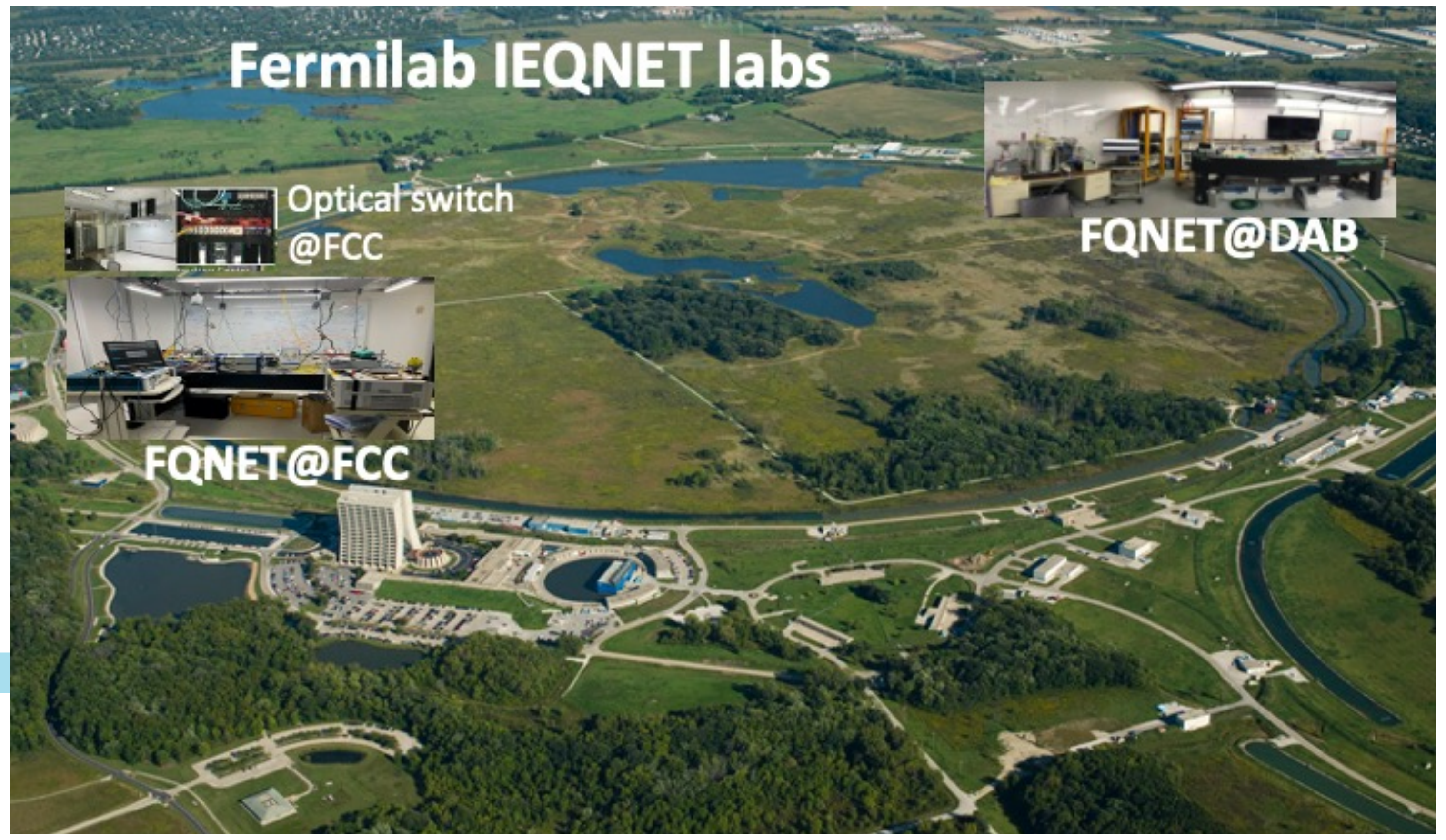
Why is quantum computing interesting for HEP?, cont.

- Quantum computing is part of a family of technologies with multiple applications:
  - ***Sensors, Computing, and Networks***
- Quantum sensors offer an ***exciting new platform for rare process and new physics searches***, e.g.
  - MAGIS-100 - new experiment at Fermilab, https://magis.fnal.gov/
  - Axion haloscopes (ADMX, HAYSTAC, etc.)
  - The Dark SRF experiment at Fermilab
  - See, e.g. https://arxiv.org/abs/2203.12714 by A. Berlin et al, https://arxiv.org/abs/2203.05375 by A. Brady et al
- The potential for quantum computers for ***quantum data analysis*** is exciting and interesting, and HEP has a large number of ***natural competencies in quantum networks*** - we are already some of the best in the world at it!

MAGIS-100

STANFORD
Fermilab
Northwestern University
UNIVERSITY OF LIVERPOOL
Northern Illinois University
JOHNS HOPKINS UNIVERSITY
SLAC
UNIVERSITY OF OXFORD
UNIVERSITY OF CAMBRIDGE
THE UNIVERSITY OF CHICAGO
GORDON AND BETTY MOORE FOUNDATION
GBMF7945
QuantiSED 2019
Science and Technology Facilities Council
UK STFC
Kavli Foundatio

Dark SRF



R. Valivarthi et al., PRX Quantum 1, 020317 (2020).

The Fermilab Quantum Institute

Fermilab Quantum Science Program Thrusts, early program

Superconducting Quantum Systems: Leverage Fermilab's world-leading expertise in SRF cavities to advance qubit coherence times and scalability of superconducting quantum systems. ***SQMS NQIA Center!***

HEP Applications of Quantum Computing: Identify most promising HEP applications on near-term quantum computers; develop algorithms and experience with state-of-the-art machines.

Quantum Sensors: Adapt quantum technologies to enable new fundamental physics experiments.

- Qubit-cavity systems for dark matter detection
- Cold atom interferometry

Quantum Communications: quantum teleportation systems and entanglement distribution architecture for connecting quantum sensors and computers

Enabling technologies: cold electronics, readout & control systems; access to quantum resources for community building and workforce development

Foundational Quantum Science/HEP connections: quantum field theory, wormholes, emergent space-time.

Slide courtesy of Panagiotis Spentzouris

Quantum computing in FQI

- ***New effort!*** Over the past three years our main focus was on exploring use cases, establishing expertise, and forming partnerships.
  - **Quantum simulation for field theory:** Foundational work on digital quantum simulation of bosons, fermion-boson interactions — PRA 98.042312 and 105.052405
  - **Quantum computing for data analysis:** Quantum annealing for galaxy morphology classification with Lockheed Martin* — https://arxiv.org/abs/1911.06259
  - **Theory inputs for DUNE:** Quantum simulation for neutrino scattering — first serious resource estimates study with U. of Washington (-> U. Trento), Los Alamos — PRD 101, 074038 (2020)
  - **Quantum computing for data analysis:** Machine learning classifiers applied to high dimensional science data with Google, Sandbox@Alphabet, University of Waterloo — Nature (npj) Quantum Information 7, 161 (2021)
  - **Advance QIS to enable HEP applications:** Qubit assignment problem (quantum computers for quantum program compilation) on Google hardware, with U. of Waterloo — under review at PRX, also https://arxiv.org/abs/2201.00445
  - **Quantum simulation for field theory:** Large scale simulation of Z2 gauge theory with Google, Sandbox@Alphabet, U. of Waterloo — Supercomputing 2021, also https://arxiv.org/abs/2110.07482
- ***In each case we leveraged FNAL expertise to advance HEP science, and built successful strategic partnerships to round our our QIS expertise and credentials.***

*This project led to Lockheed's participation in the NQIA Center hosted at FNAL (SQMS)

Explore and identify HEP science applications

Leverage Fermilab strengths

Utilize strategic partnerships to fill gaps

Advance quantum technologies

Strategy and tactical approach for FQI

- **Illustration by example** — simulating Z2 gauge theory: paper at Supercomputing 2021 (Workshop on Quantum Computing, see also https://arxiv.org/abs/2110.07482)
  - Largest classical simulation of Z2 on a quantum device to date at 36 qubits.
  - **Enabling HEP science:** direct study of the bounds for quantum advantage in QFT; 6x6 qubit grid was insufficient for the science, likely require at least 7x7 (theoretically possible to simulate classically, but ~exascale-sized)
  - **Leveraging HEP and Fermilab competencies:** Theory expertise in problem and quantum circuit design, SCD experience with large scale distributed computing
  - **Advancing QIS where appropriate:** noise model parameter scan to inform the next generation of QPUs - where do various improvements have the most impact?
  - **QIS partnerships to fill expertise gaps:** work with experts at Google, Sandbox@Alphabet, and University of Waterloo to model quantum noise, improve quantum circuits, and accelerate applications on ASIC simulators (TPUs)
    - *This project was not on a QPU — but the relationship with Google was based on participation in their Early Access Partners program to use their Sycamore QPU (quantum advantage demonstration chip).* ***Special thanks to Google and Sandbox@Alphabet for donating cloud computing and TPU time for this research!***

Simulating Z2 gauge theory

- We would like to understand the boundaries for useful "scientific advantage."
- This means pushing the *classical simulation* of quantum systems as far as we can.
- We also need to understand whether *Quantum Error Correction (QEC)* is required to solve HEP problems.
- We ***studied Z2 gauge theory on a simulated version* of Google's Sycamore QPU with a large noise scan.***
  - Square lattice connectivity is a natural map for Z2 gauge theory.
  - We built a realistic parameterized quantum noise model and performed a large scan over parameter space in order to understand the relationship between theory and hardware errors.

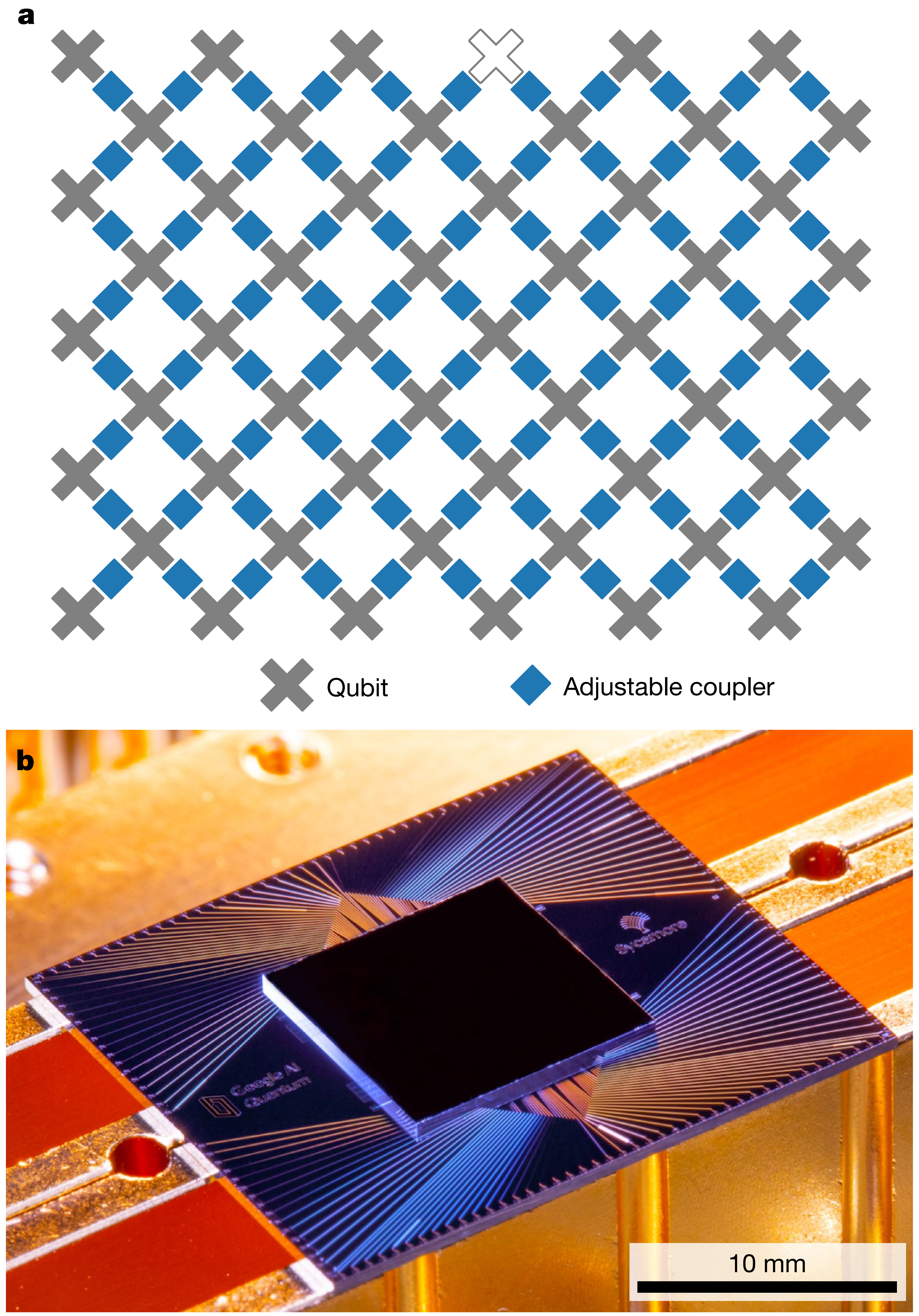


Fig. 1 | The Sycamore processor. a, Layout of processor, showing a rectangular array of 54 qubits (grey), each connected to its four nearest neighbours with couplers (blue). The inoperable qubit is outlined. **b**, Photograph of the Sycamore chip.

Arute et al, Nature 2019, https://doi.org/10.1038/s41586-019-1666-5

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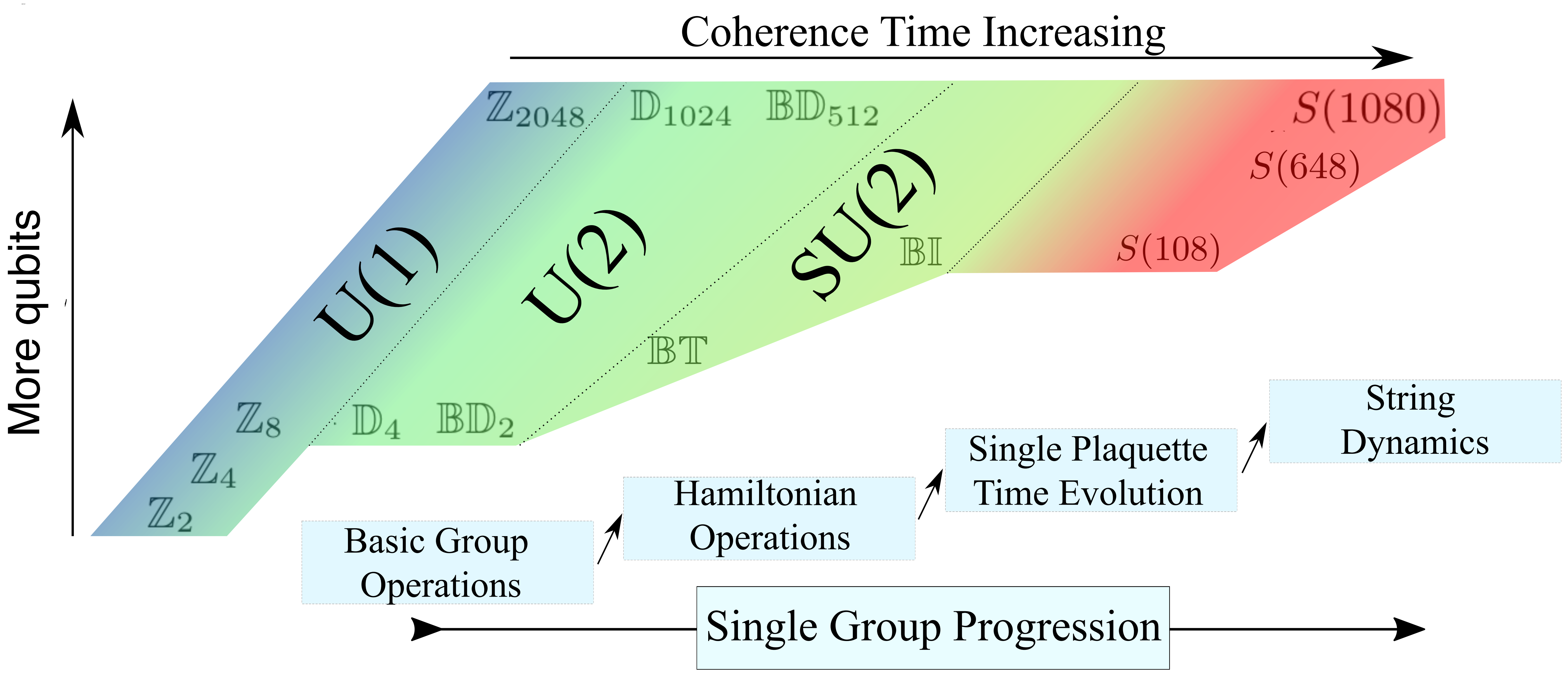
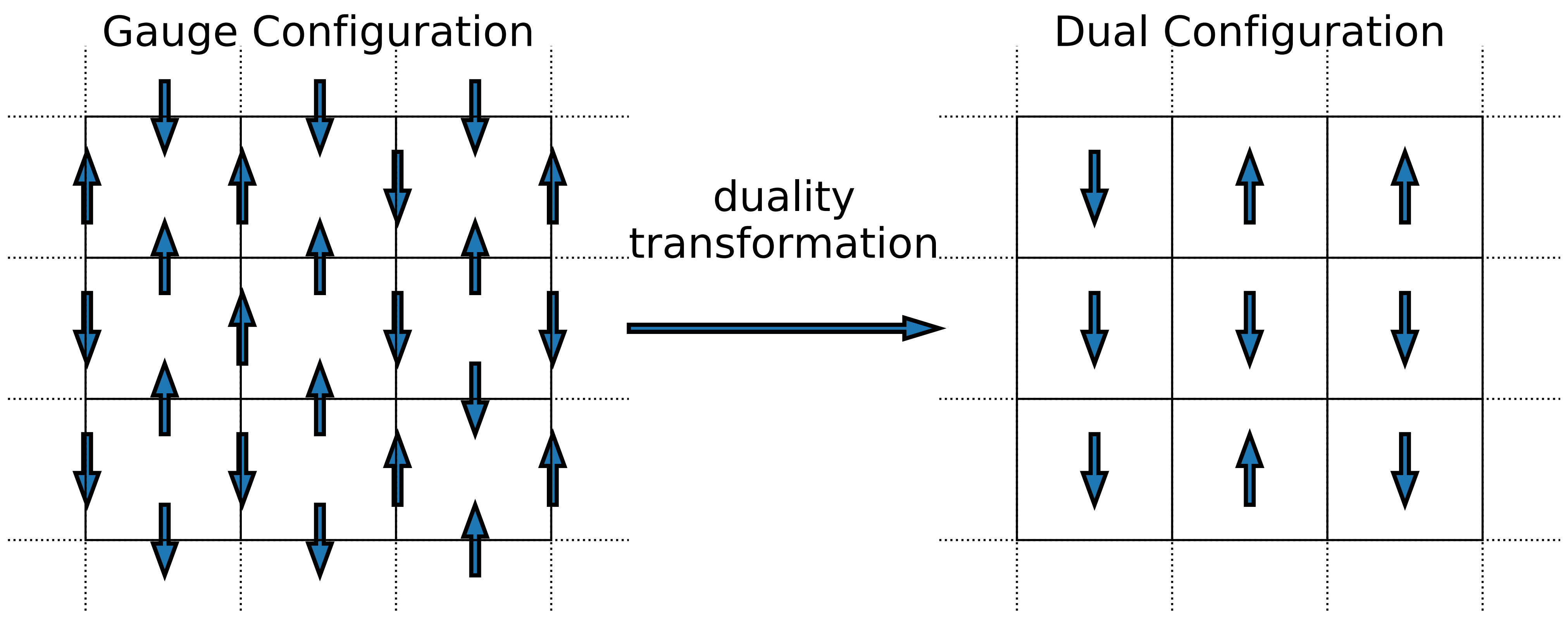
*The simulated QPU was modified to admit a 6x6 qubit lattice.

Approximating continuous gauge groups

- Lattice field theory places the theory on a lattice in a finite volume. Ultimate goal is full QCD with time evolution - exponentially expensive on classical computers.
- Perform computations at different lattice sizes and spacings and extrapolate to the continuum.
- Here - use a duality transformation: Z2 gauge action becomes the Transverse field Ising Hamiltonian. Same physics for half the qubits.

$$\hat{H}_{\text{dual}} = -\frac{\gamma}{\beta_H}\sum_{\vec{n},\hat{\mu}} \hat{\sigma}^x_{\vec{n}}\hat{\sigma}^x_{\vec{n}+\hat{\mu}} - \gamma\beta_H \sum_{\vec{n}} \hat{\sigma}^z_{\vec{n}}$$





Figures courtesy of H. Lamm, E. Gustafson, E. Peters

Observables and convergence

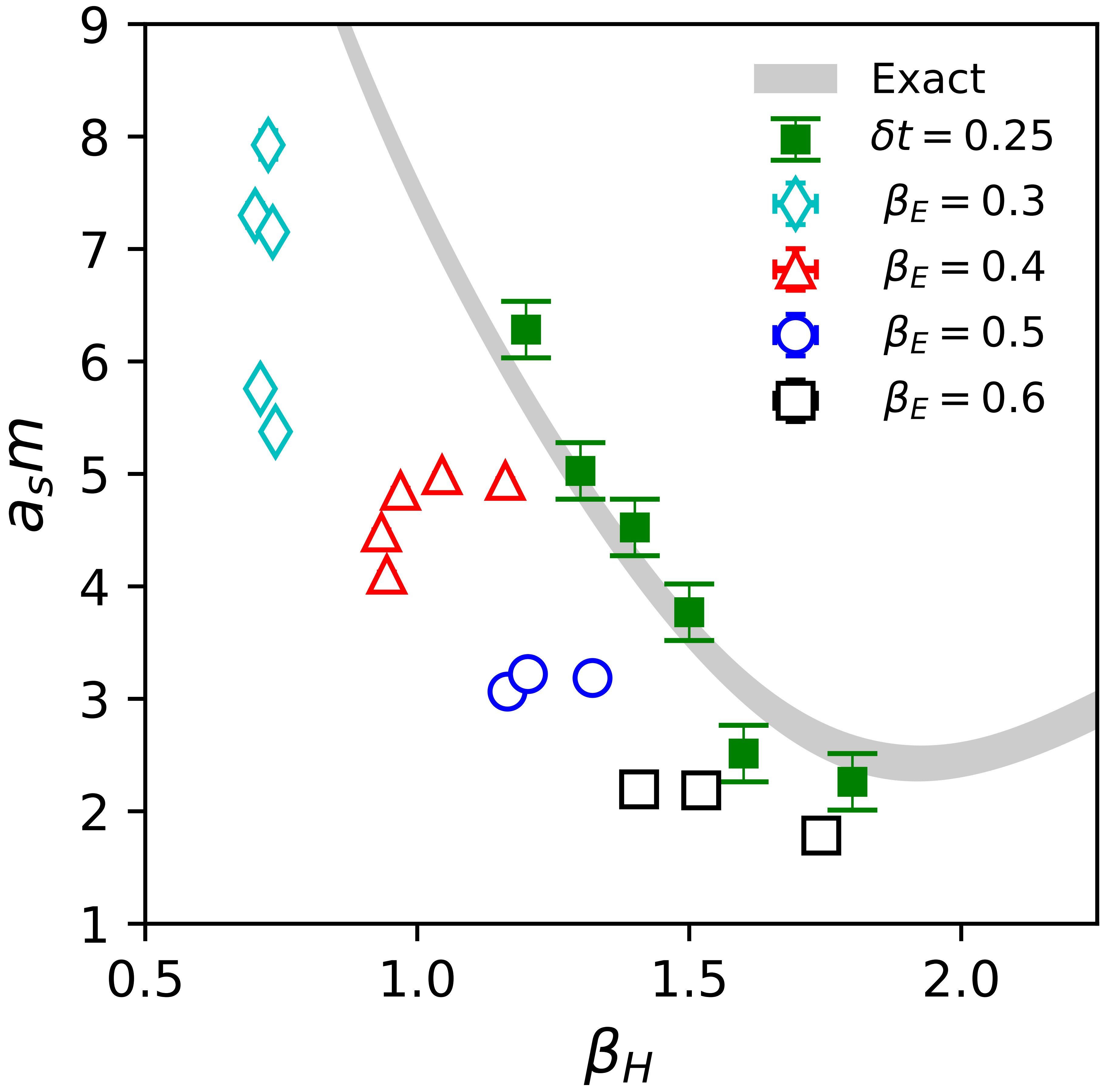
- The observable is a correlator between sites - simulate ***time evolution*** -> the Fourier transform gives the **glueball mass**.
- ***We chose an observable that is NOT sensitive to sign problems so we may compute the exact result classically*** - we may ***use the errors to gauge what the likely errors would be on a quantity we need a quantum computer for.***

$$\mathcal{C}_{i,s}(t) = \langle\Omega|\hat{U}^\dagger(t)\hat{X}_i\hat{U}(t)\hat{X}_s|\Omega\rangle.$$

$$\hat{U}(t) = \sum_E |E\rangle\langle E|e^{-itE}.$$

Time evolution eigenbasis expansion

$$\mathcal{C}_{i,s}(t) = \sum_{\{E_k\},\{E_m\}} A_{i,s}(E_k, E_m)e^{it(E_k - E_m)},$$



E. Gustafson et al, https://arxiv.org/abs/2110.07482

Fig. 1. Comparison of the lattice glueball mass $a_s m$ as a function of β_H obtained from: (grey band) extrapolating the exact diagonalization of $\hat{H}$ from smaller volumes, (open symbols) classical simulations at fixed β_E and varied ξ, (closed symbols) quantum simulations at fixed δt for various β_H.

$$\beta_E/\xi = \sqrt{\beta_H}e^{-\beta_E \xi}$$

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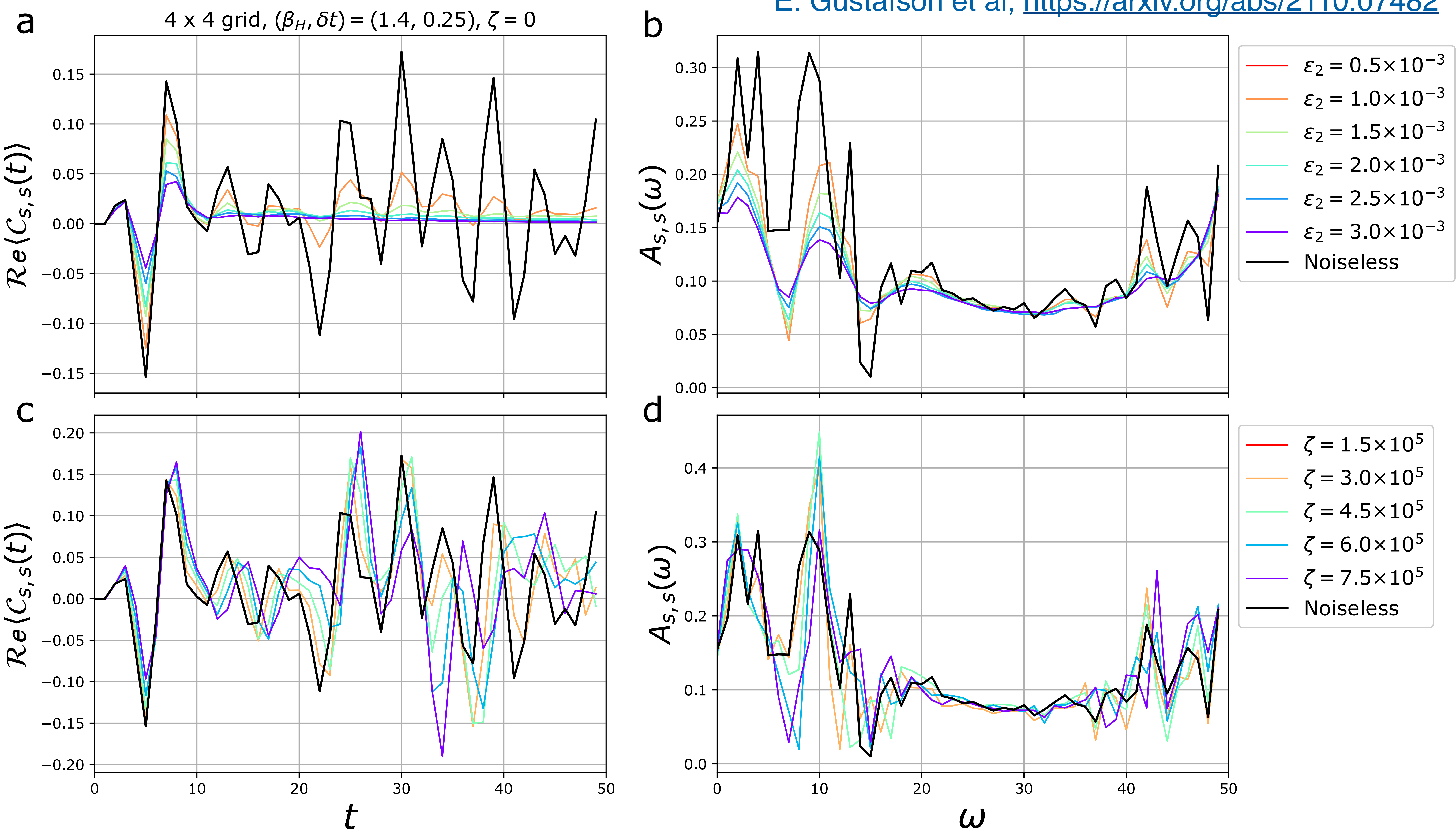
Simulation deliverable is a time series

E. Gustafson et al, https://arxiv.org/abs/2110.07482

- For each n x n qubit lattice (3x3, 4x4, 5x5, 6x6) and parameter set (β_H,δt,ε,ζ) we compute the $C_{i,s}(t)$ time series.
- $O(n^2)$ local observables
- Fourier transform -> spectrum -> glueball mass (mass gap) $E_1 - E_0$



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Simulating large lattices

- Large (e.g. 6x6, and even 5x5) face ***severe memory and speed constraints***.
- Noisy simulation is not even possible for 6x6 lattice (memory requirements would only fit on a leadership class supercomputer, using the whole machine).
- ***Very large speed-up possible on Google TPUv3 ASIC chips*** (linear algebra accelerators designed for machine learning workloads) using private codes.

4 TB RAM

Platform	6×6
m1-ultramem-160 (qsimcirq)	470 hours
m1-ultramem-160 (qsim)	295 hours
TPUv3-512	4.5 hours

qsimcirq - 37 qubits, 2-local oservables

qsim, TPU - 2 x 36 qubits, 1-local observable

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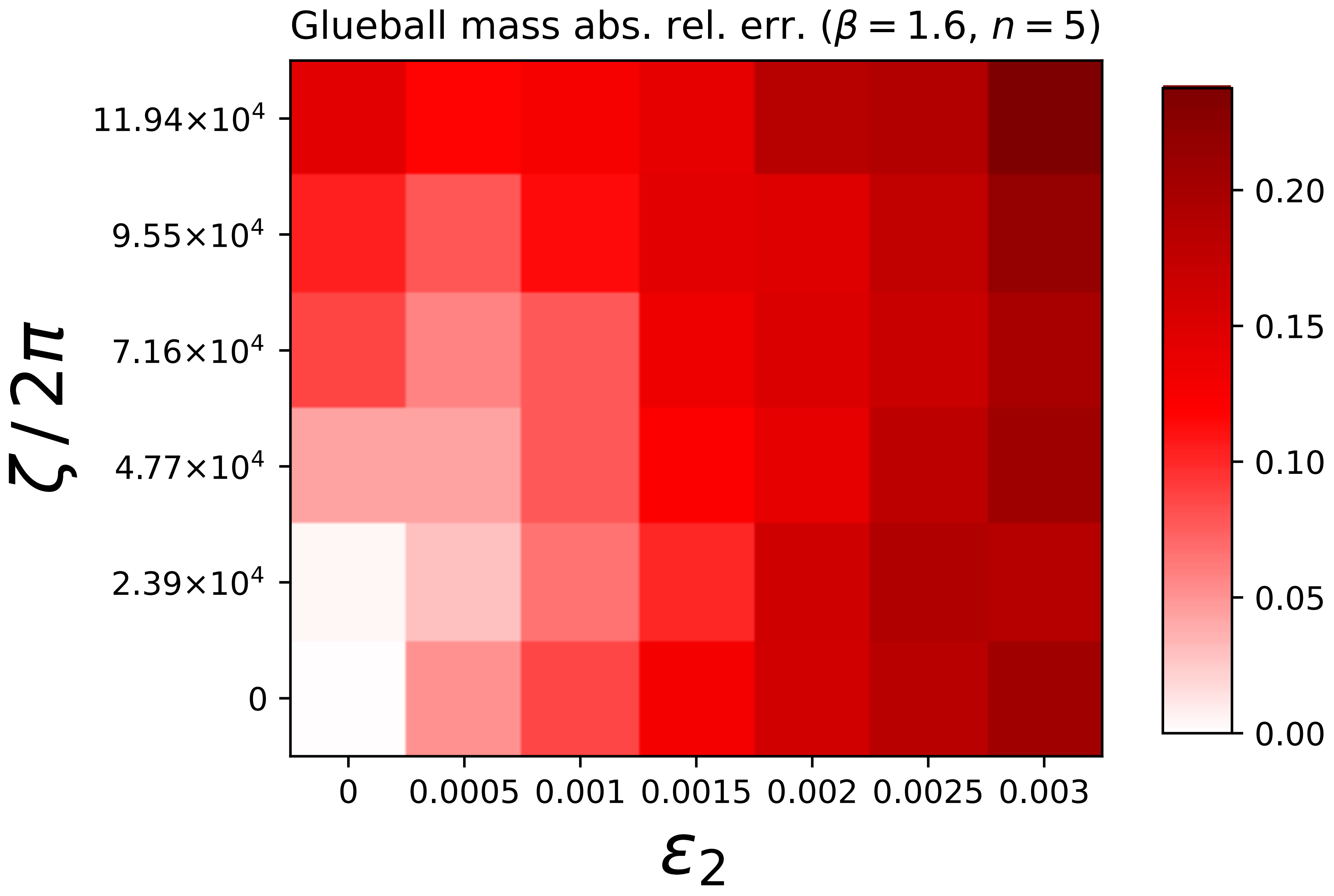
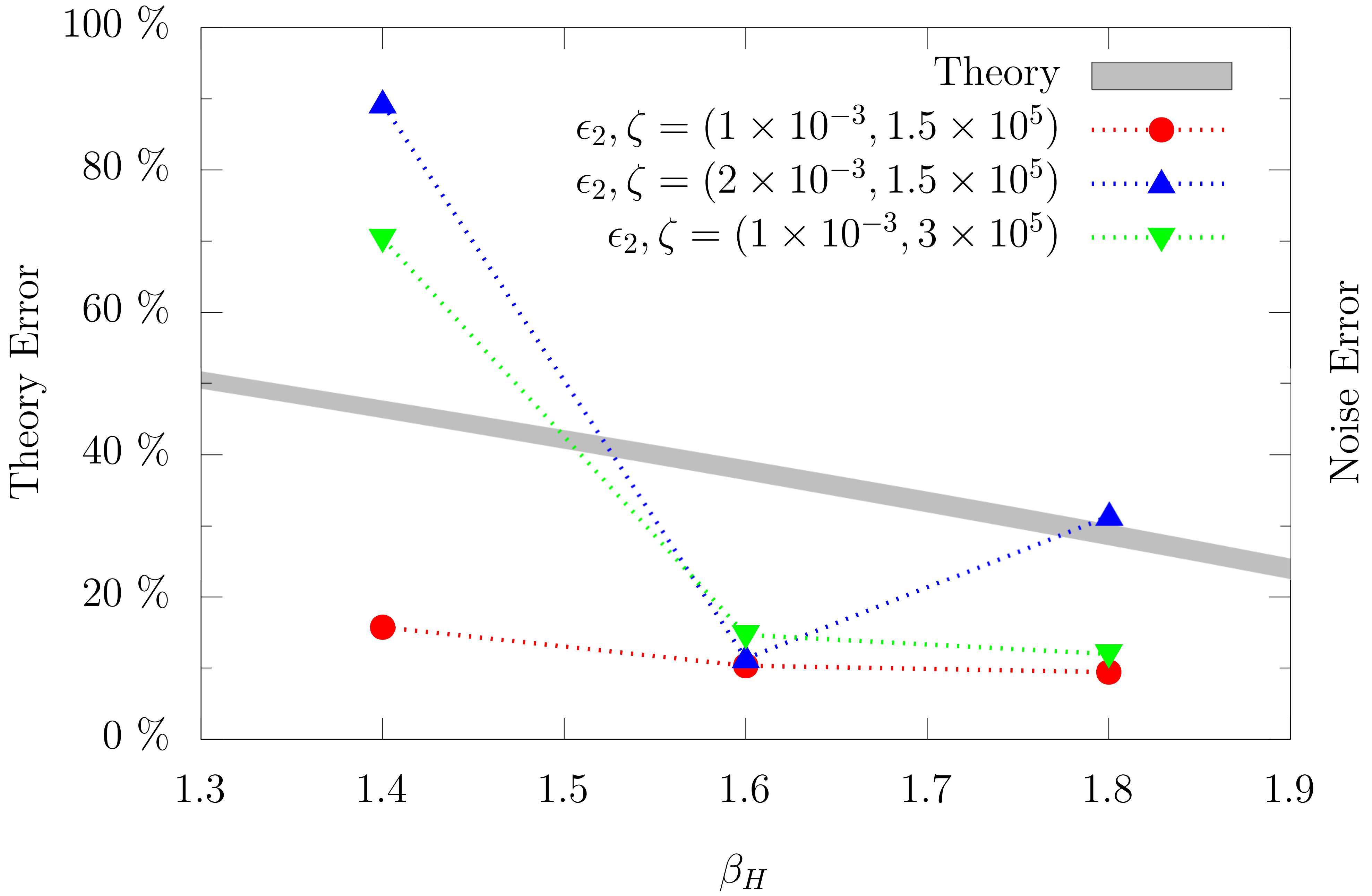
Theory errors and noise errors

- Large amount of data to analyze! Representative example:
  - 5 x 5 lattice noise sweep - (6 ζ's) x (6 ε_2's) x (3 β_H's) x (1 δt)
- Compare errors from noise to theory errors.
- ζ, ε_2 values better than current hardware state of the art by x10-100
- Results here were computed using 64 Nvidia V100 GPUs in parallel on Google Cloud Platform (500 GPU-hours for the plot on the left)





Study conclusions

- Even with results up to 6 x 6 in lattice size, the glueball mass has a high uncertainty.
- ***Observables of interest for quantum advantage will likely require at least a 7 x 7 lattice to be included, perhaps larger - right at the edge of what we can simulate exactly with exascale resources.***
  - ***Need to better understand the interplay between inexact simulation and theory errors!***
- **Noise errors were found to be comparable to physics theory errors**, but this was ***assuming roughly x10-100 better qubit noise*** parameters than what we have in modern hardware.
- Great success partnering with scientists at Google and Sandbox@Alphabet
- We helped write on a tutorial if you'd like to try the cloud platform 🙃
  - https://cloud.google.com/architecture/quantum-simulation-on-google-cloud-with-cirq-qsim

FQI Quantum Algorithms: Vision and objectives

- What are the **goals for the next 5 years?**
  - It is clear one of the strongest early applications will be quantum simulation of field theories. Data analysis for quantum sensors, possibly networked, to extend and enhance New Physics searches is another promising candidate.
    - ***These two are likely to be our main focus.***
  - Quantum computers are plausibly on track to enter the era of Quantum Error Correction (QEC - think of it as “self healing” for decoherence) by the end of the decade. This will enable calculations of real scientific value to HEP. There are a ***number of important open questions***:
    - Will commercial devices be well-suited to run our applications or will they focus on, e.g. quantum chemistry and materials problems with stronger support in the business community?
    - What *are* the requirements for a quantum computer for HEP applications?
    - What is the most effective role we can play in enabling, and shaping the contours of, QEC?

Vision and objectives moving forward, cont.

- What are the goals for the next 5 years?
  - Historical analogies can be dangerous, but the lattice computing trajectory is compelling. ***We will engage in a co-design process to define the computing requirements for HEP physics and find and defend the "boundaries" of quantum advantage.***
  - We will also ***work to better understand the interplay between quantum networks, sensors, and algorithms.*** The line is blurry - the same devices can often be used for sensing and computation!
    - ***These two goals leverage HEP and especially Fermilab's strengths in quantum field theory, quantum algorithms, superconducting devices, quantum networks, detector instrumentation, and theory support for new physics searches.***

Thanks for listening!

Noise models and hardware viability

- We built a noise model with two parameterized components.
- Local depolarizing noise - rough model for gate infidelity, where P_j is a *k*-local Pauli operator (e.g., for bit flip and phase errors) and p(j) is a function of ε (governs the likelihood of a given Pauli operator or the identity.)

$$\mathcal{D}_n[\epsilon](\rho) = \sum_{j \in \{0,1,2,3\}^n} p(j) P_j \rho P_j$$

- We apply D_1 to qubits after applying a single-qubit gate and D_2 after applying a two-qubit gate, with $\varepsilon_2 = 10\ \varepsilon_1$.
- For qubit-crosstalk, we use a unitary ZZ error*, with a parameter ζ based on fabrication defects

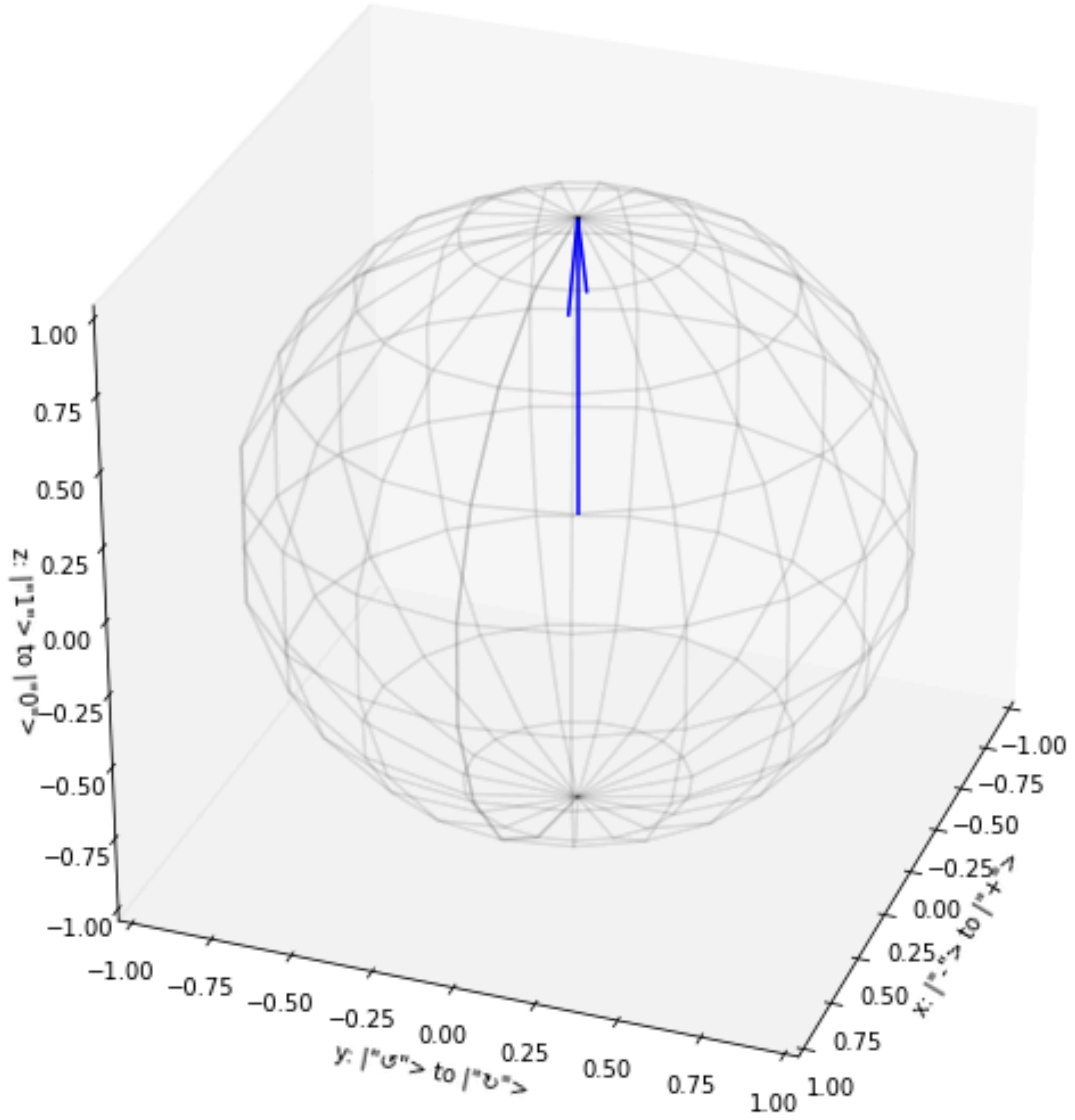
$$U_{ZZ}[\zeta] = \exp\left(-i2\pi\zeta T |11\rangle\langle 11|\right)$$

*See, eg. D. McKay in PRL 122 (May 2019)

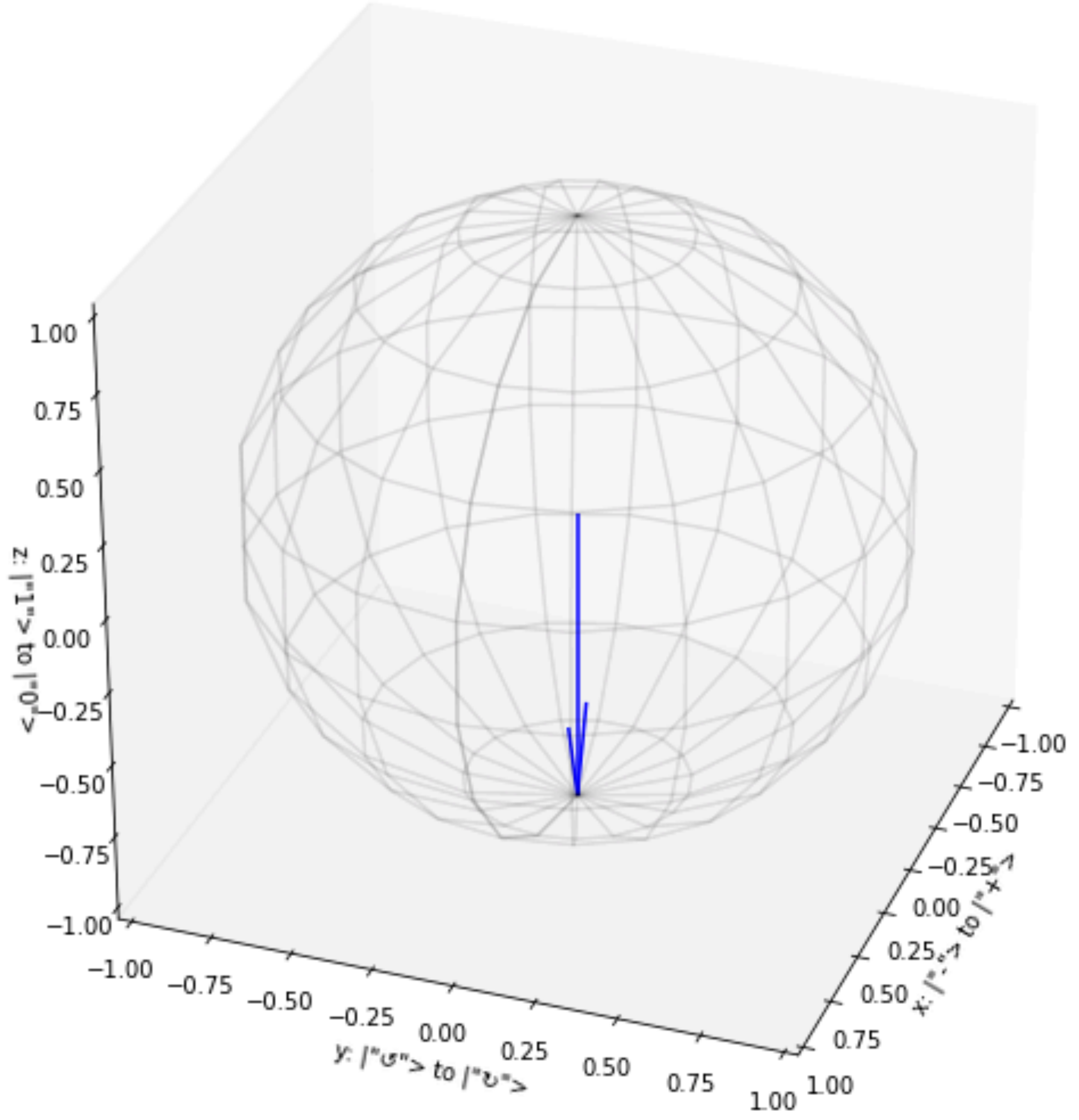
Qubits

$$|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \alpha \times \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta \times \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv \alpha|0\rangle + \beta|1\rangle$$

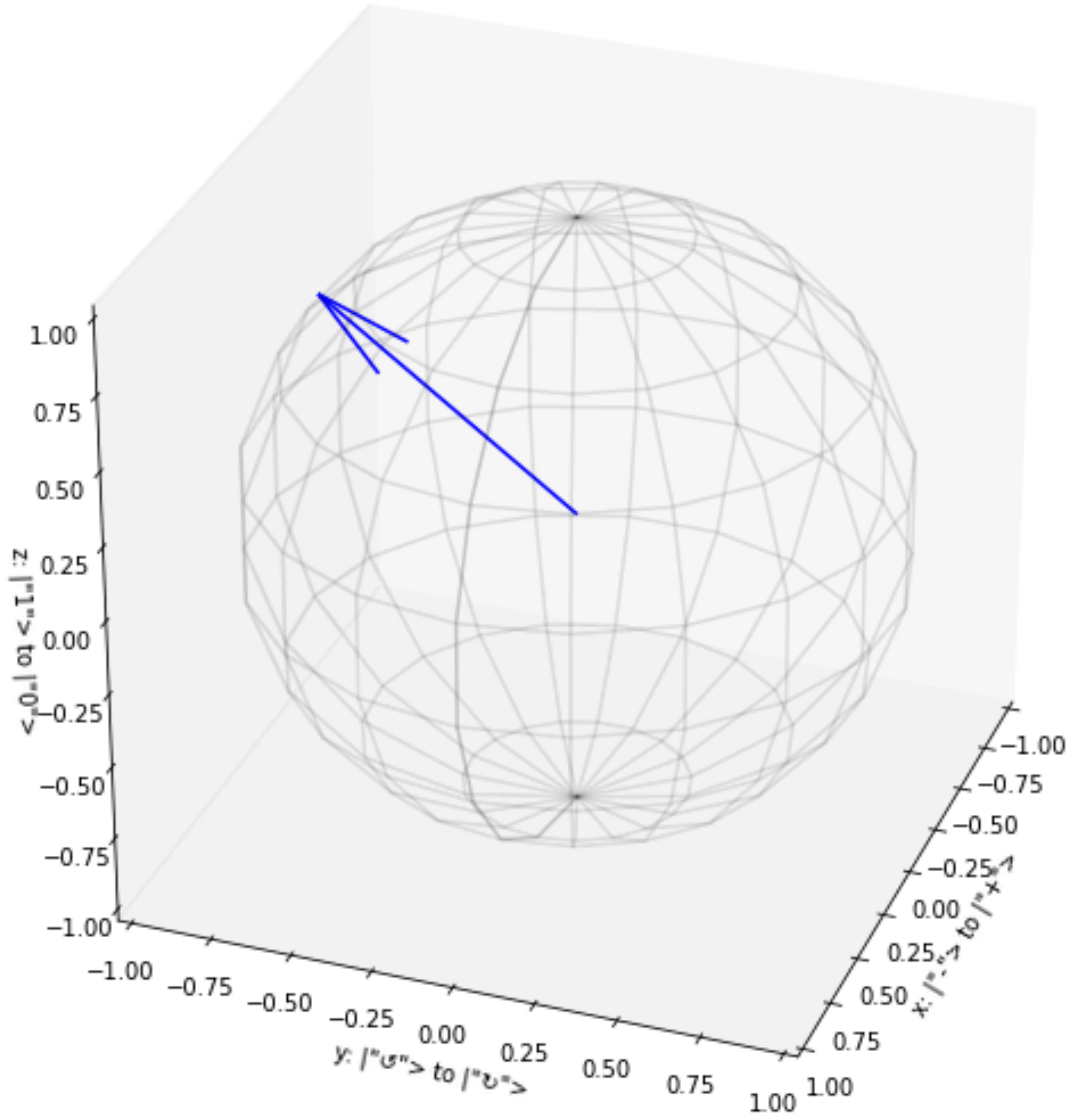
Quantum operators rotate the vector's direction.



$|0\rangle$



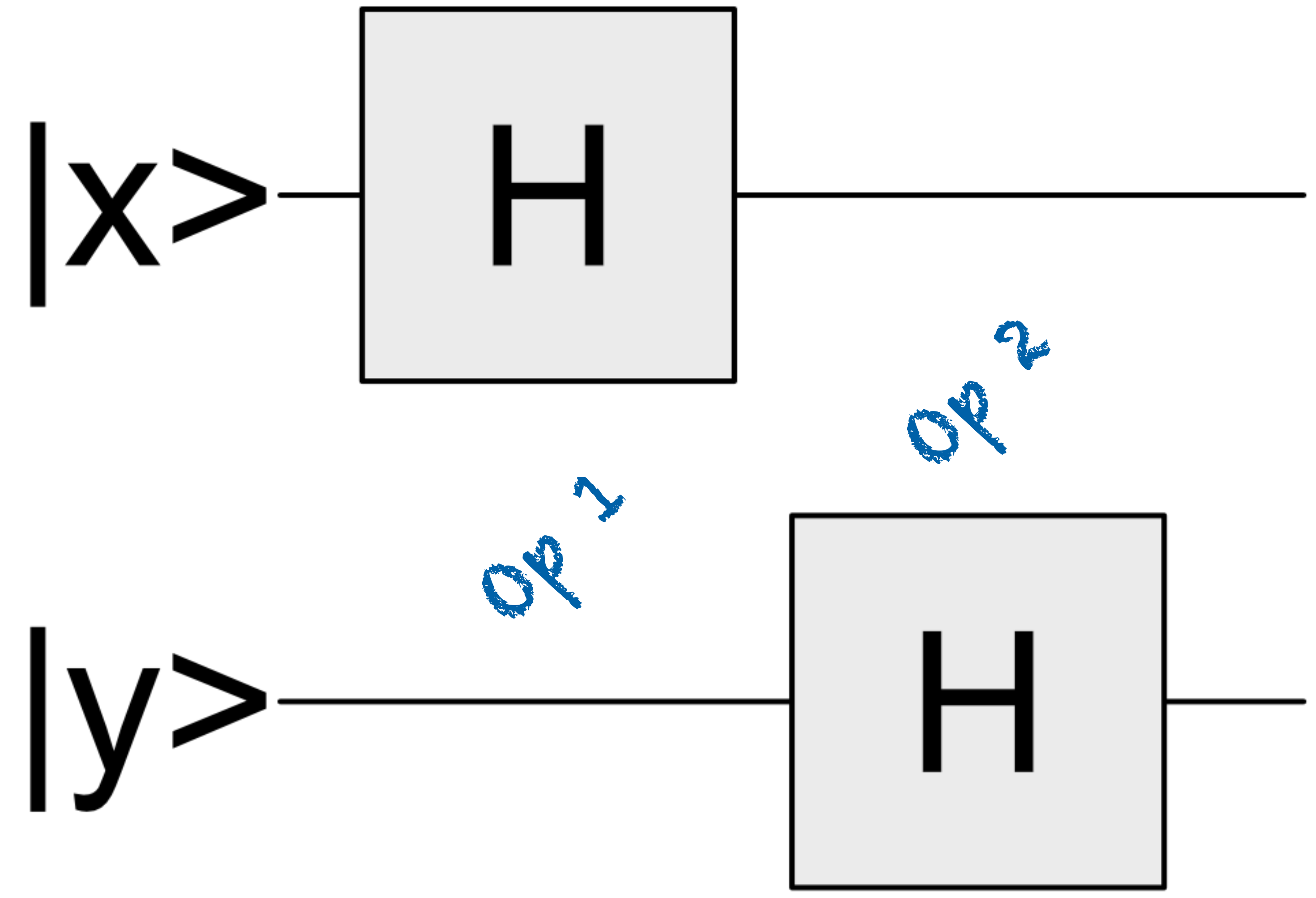
$|1\rangle$



$\sqrt{0.2}|0\rangle + \sqrt{0.8}|1\rangle$

What *is* quantum computing?

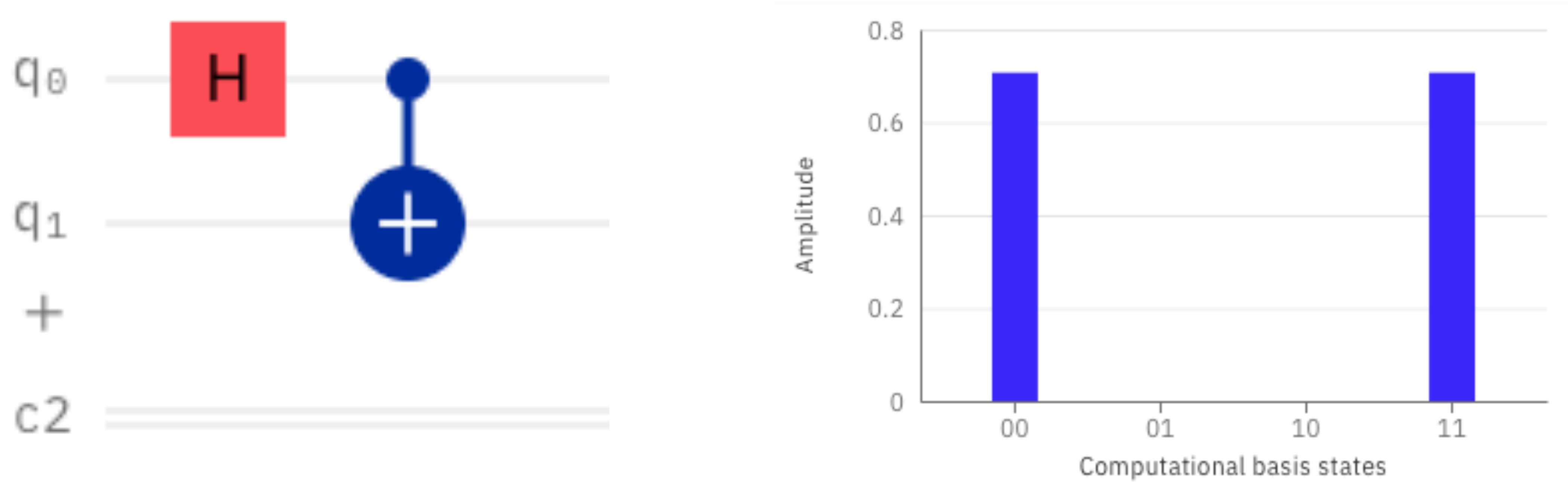
Circuit composer: https://quantum-computing.ibm.com/

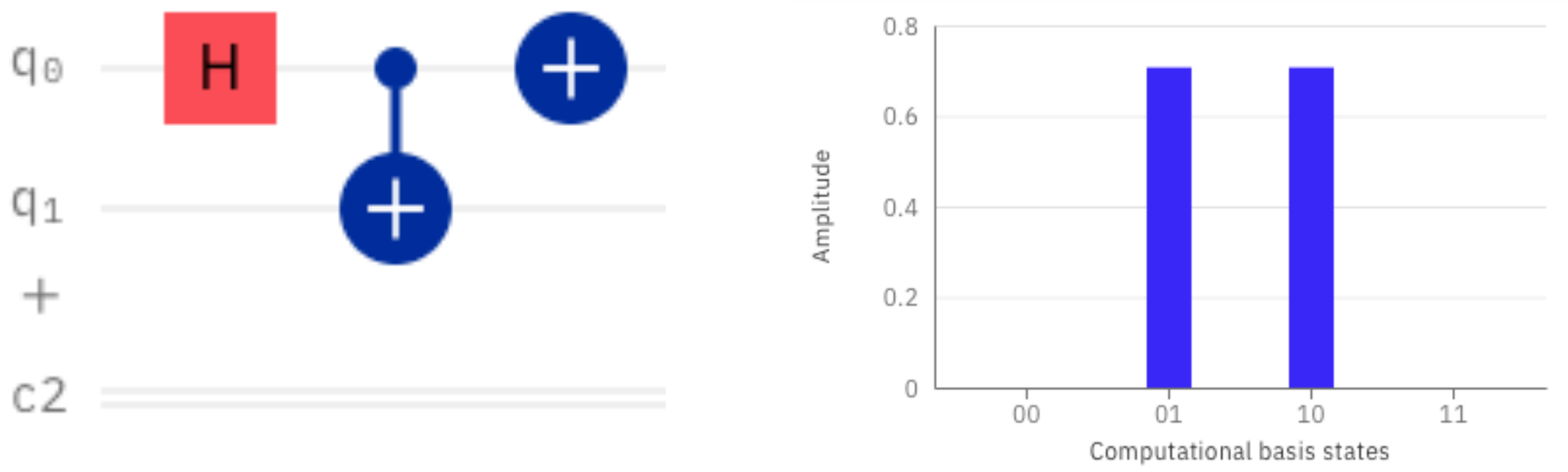


$$H \otimes I \qquad\qquad I \otimes H$$

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix}$$

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \rightarrow \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{2}\left(|00\rangle + |01\rangle + |10\rangle + |11\rangle\right)$$





Super hand-wavy "quantum advantages"

- Superposition lets us create a sum state with two operations instead of four.
- Entanglement means we can manipulate the entire state vector with one operation.
- *Exploiting* these operations with *provable* speedup is actually pretty hard! (Consider measurement if nothing else…)

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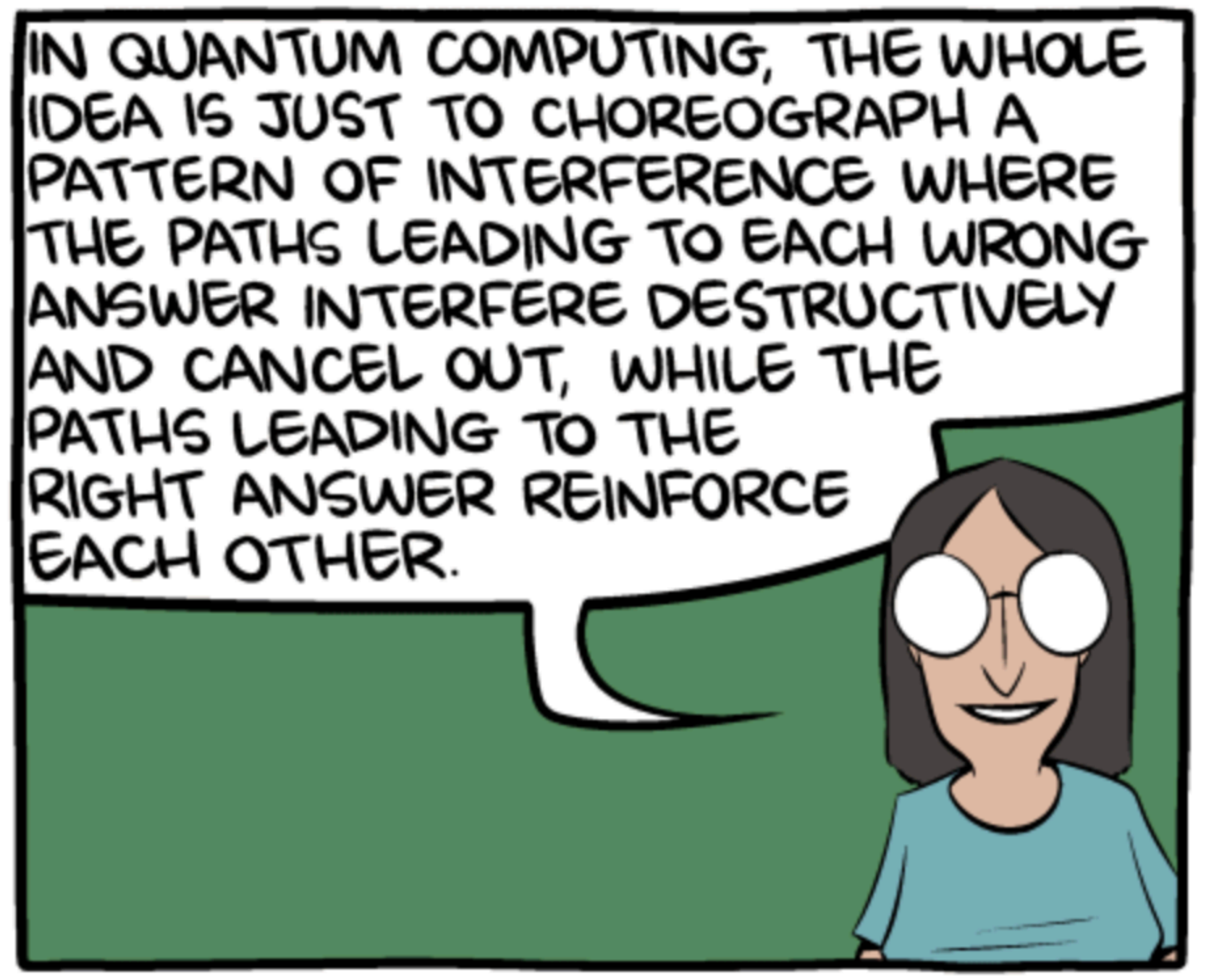
What is quantum computing *good for?*

Photo by Erik Lucero, Google

- Many things (cryptography, communications, etc.), but the "commercial killer app" will probably be the first proposal*: the simulation of quantum systems - and the money is in chemistry now. Quantum computers will ultimately be able to do something classical computers will never be able to do - simulate exactly the behavior of molecules with complex electron behavior.
- The physics undergirding this is that of a system of interacting fermions.
- There are fewer commercial applications in the simulation of, say, nuclear matter in neutrino-nucleus scattering, but we can benefit from the commercially motivated research in quantum chemistry a great deal!
- Why is quantum computing powerful?
  - https://www.smbc-comics.com/comic/the-talk-3



* R. P. Feynman. Simulating physics with computers. *International Journal of Theoretical Physics*, 21(6):467–488, Jun 1982.