Quantum Information Science at Fermilab

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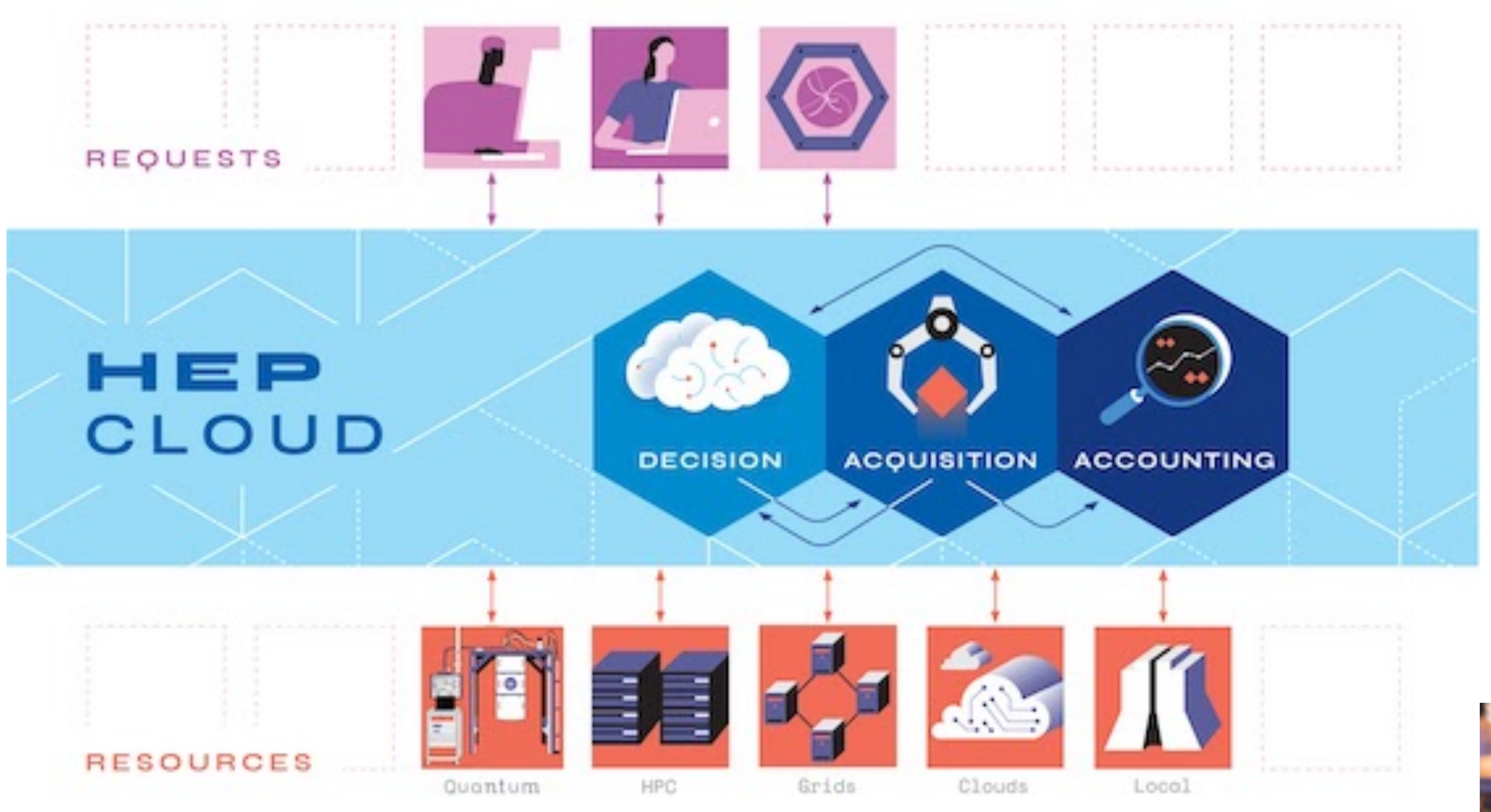
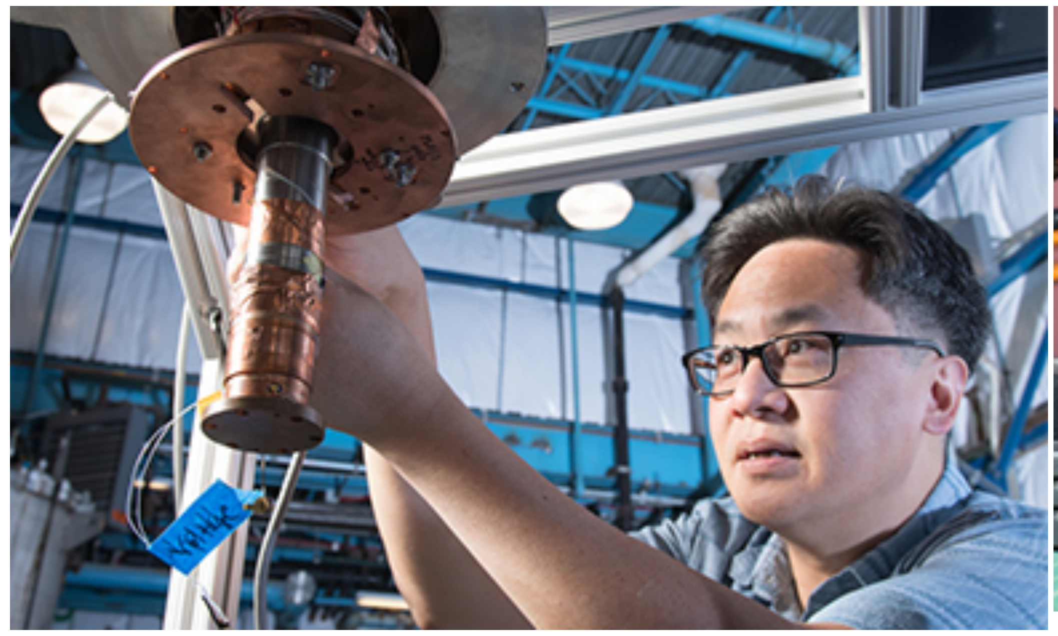
University of Liverpool HEP Seminar
2021-January-27

Overview

- What is quantum computing?
- Quantum computing at Fermilab: New organizations
  - The Superconducting Quantum Materials and Systems Center
  - The Fermilab Quantum Institute
- Applications of quantum computing
  - Neutrino scattering
  - Why is this problem so hard?
  - Current work

SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER





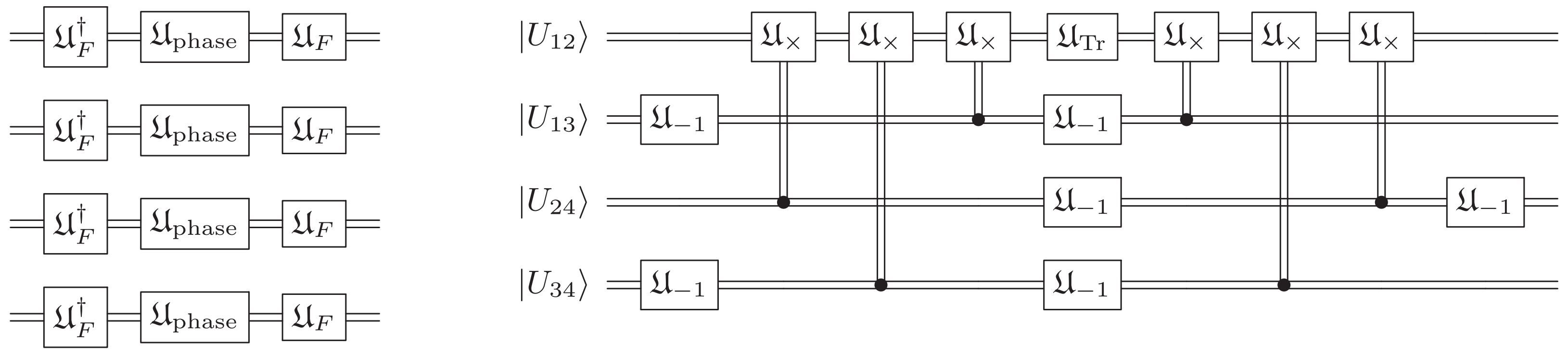


FIG. 1. Circuits for the propagation of a pure-gauge lattice field theory. The first circuit implements $\mathcal{U}_K^{(1)}$ on four links (in general, L links are needed). The second circuit shows the application of $\mathcal{U}_V^{(1)}$ to a single plaquette $\mathrm{Re\,Tr}\, U_{13}^\dagger U_{34}^\dagger U_{24} U_{12}$, and must be applied to every plaquette in the theory. Note that in these circuits, we use a doubled line to represent a G-register, rather than a single qubit.

LAMM, LAWRENCE, and YAMAUCHI PHYS. REV. D **100,** 034518 (2019)

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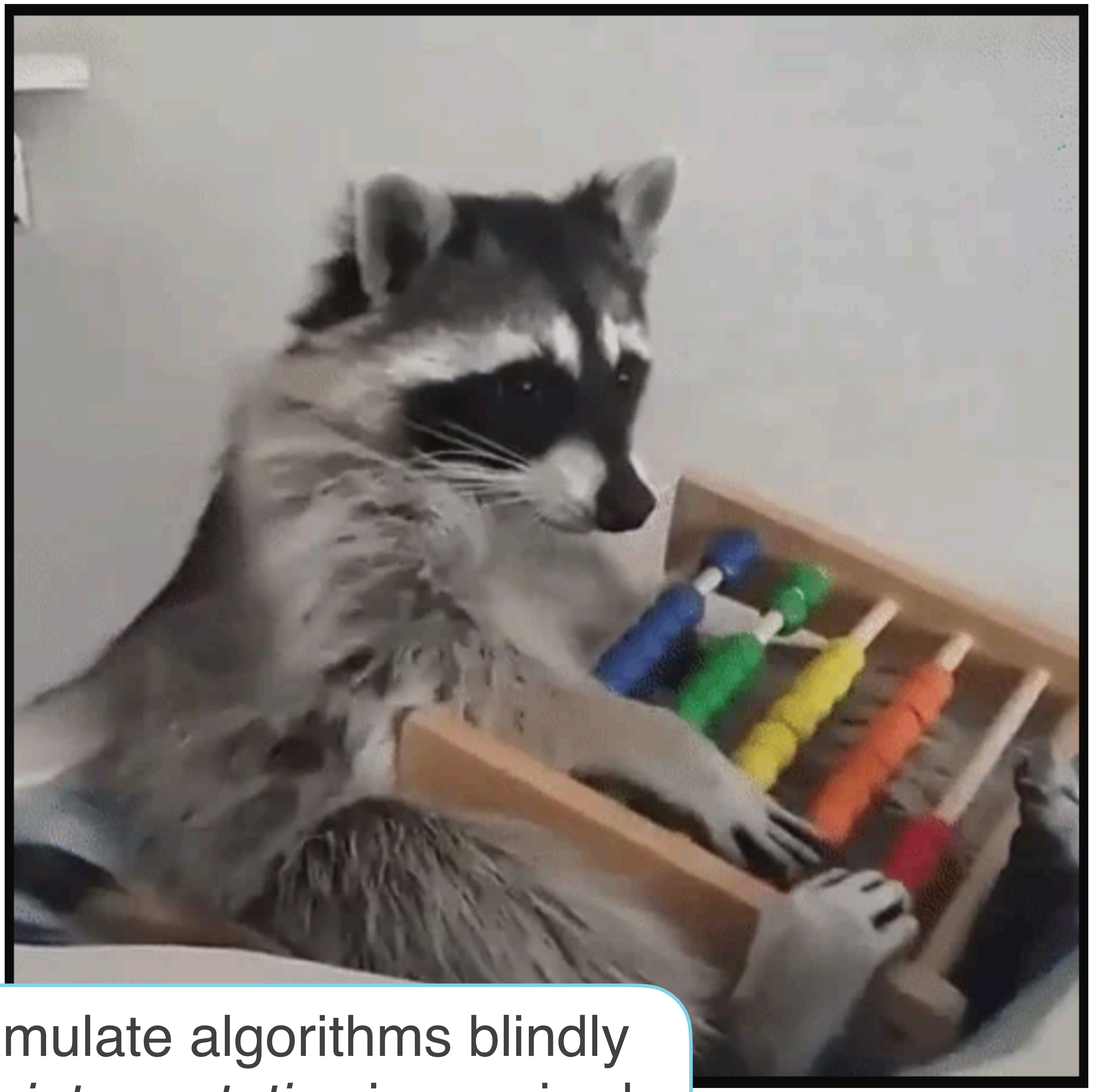
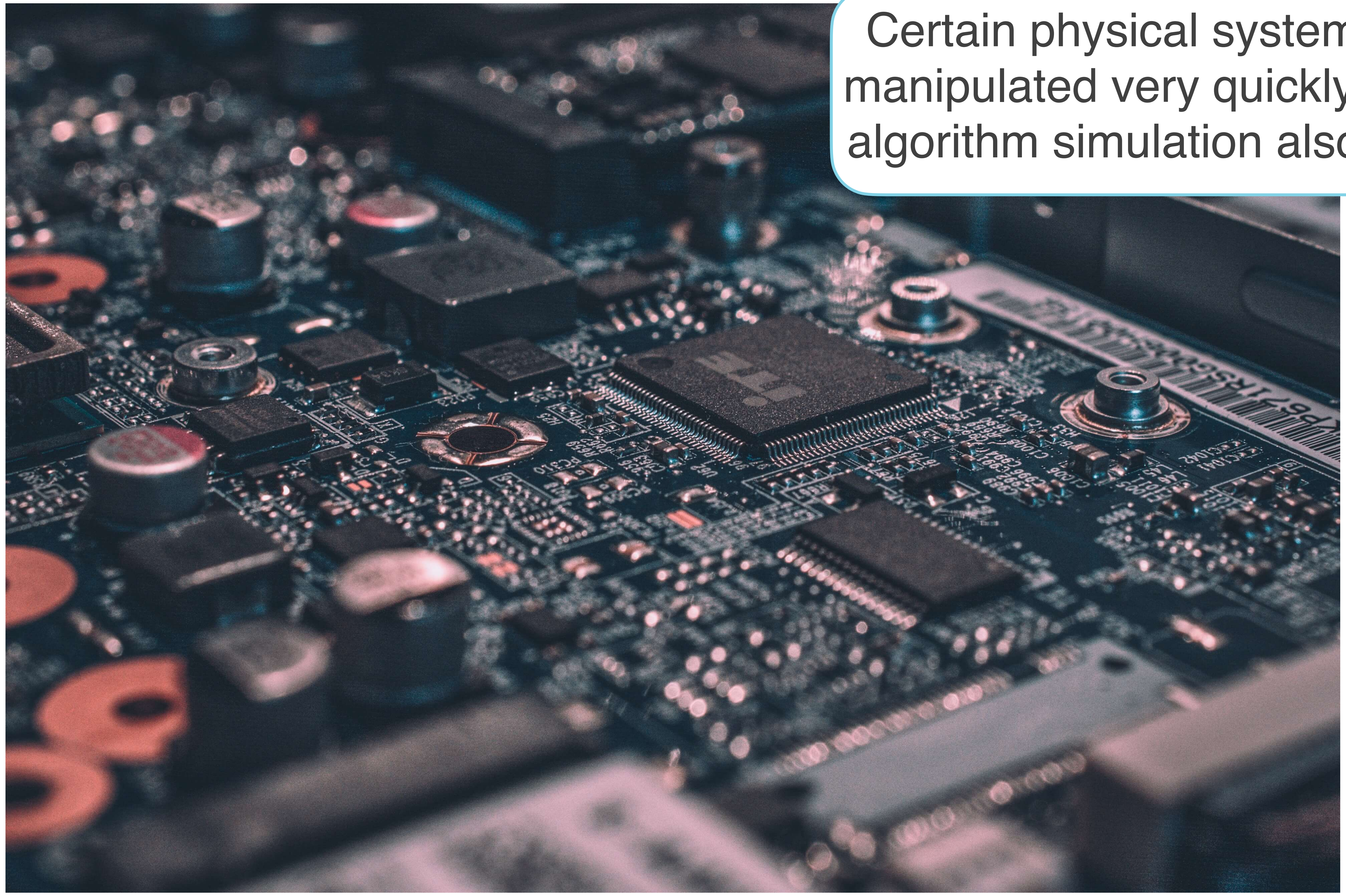
What is computing?

- 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.

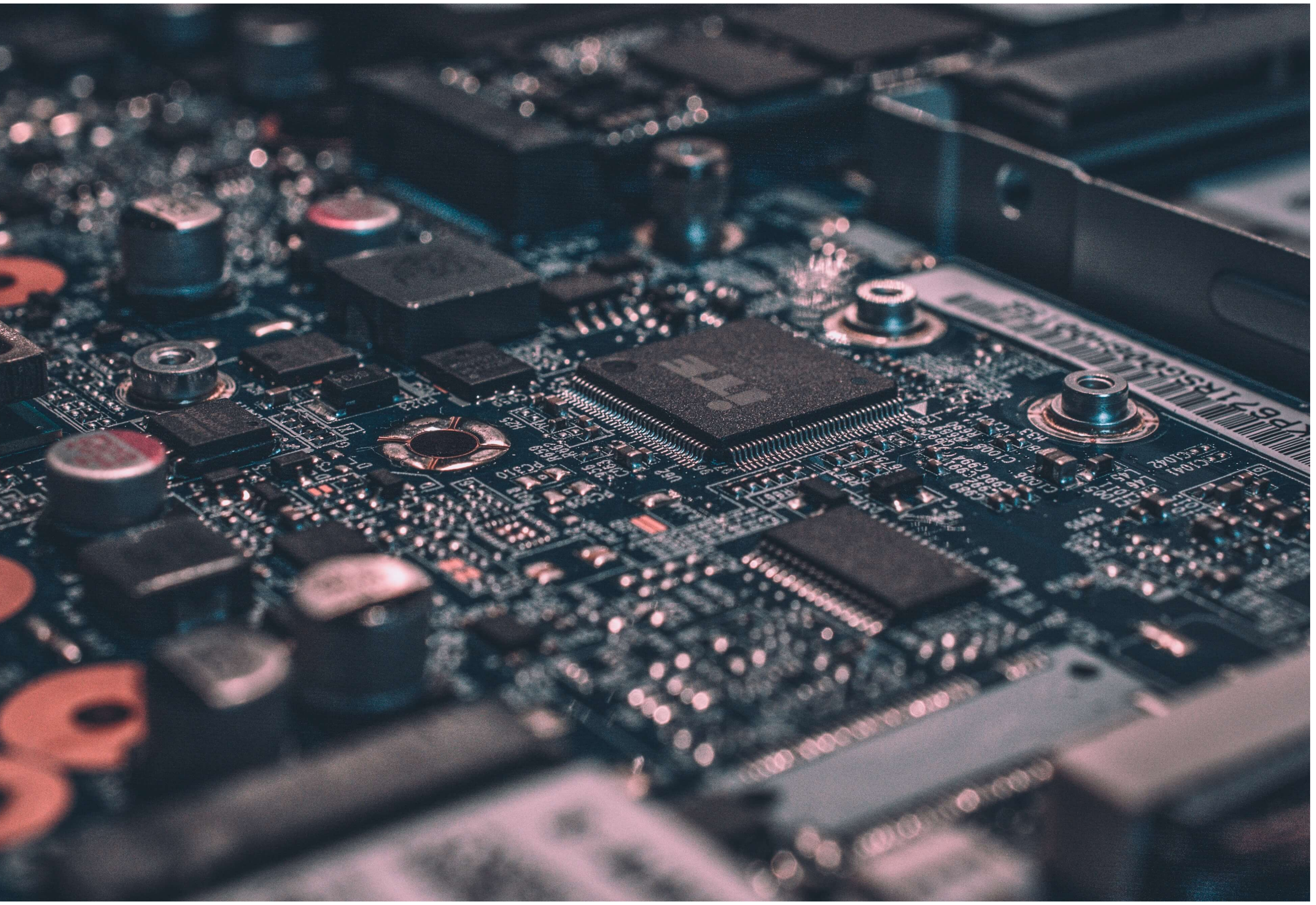




Certain physical systems can be manipulated very quickly - making algorithm simulation also very fast.

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

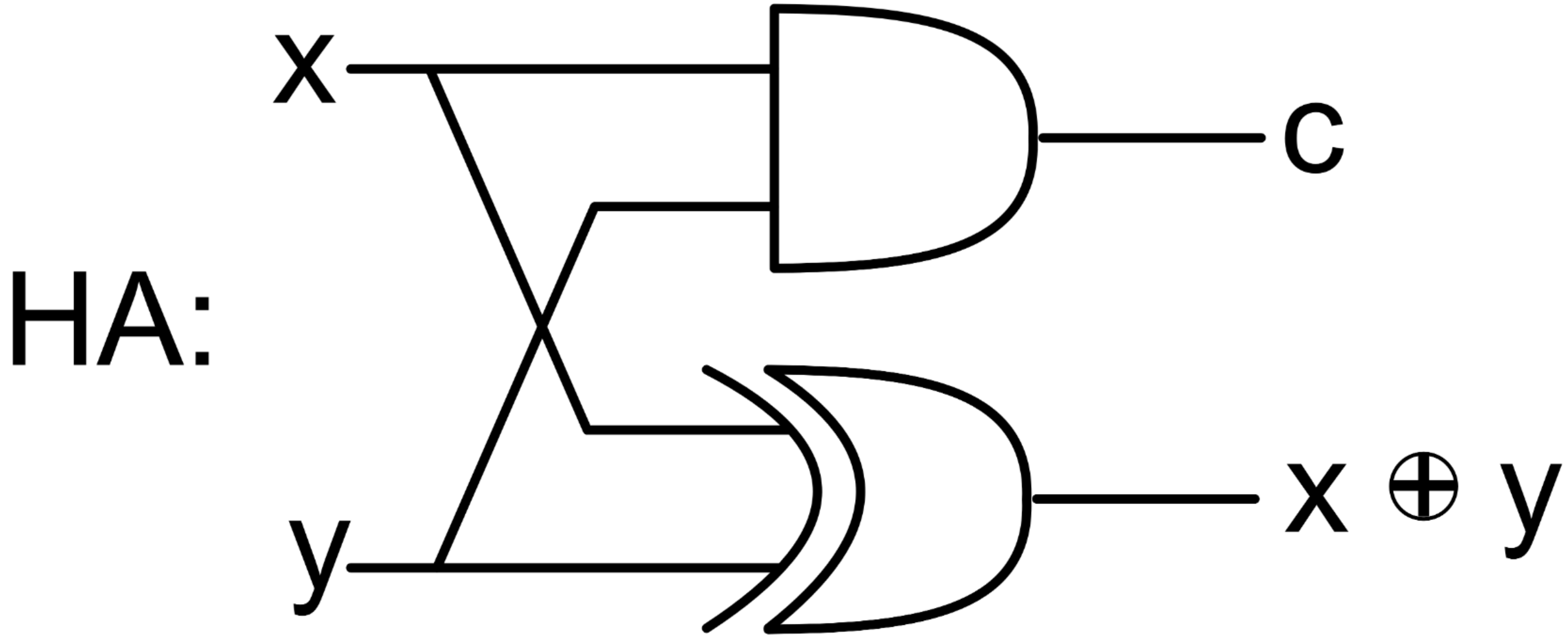
What is classical computing?

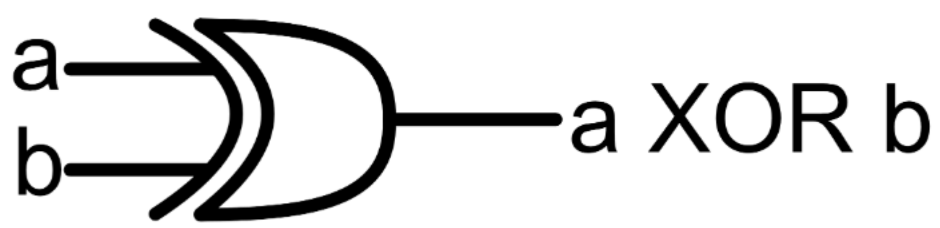


You can see how you would implement a table like this one with logic gates:

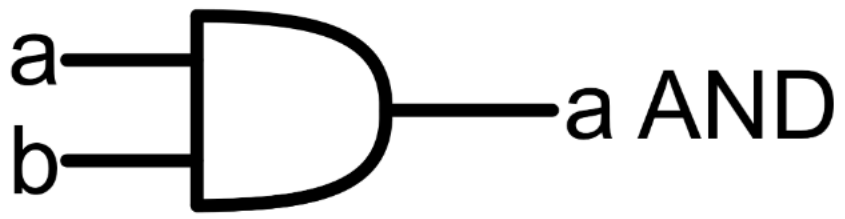
```
  0     0     1     1
 +0    +1    +0    +1
 ---   ---   ---   ---
 00    01    01    10
```

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





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



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

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

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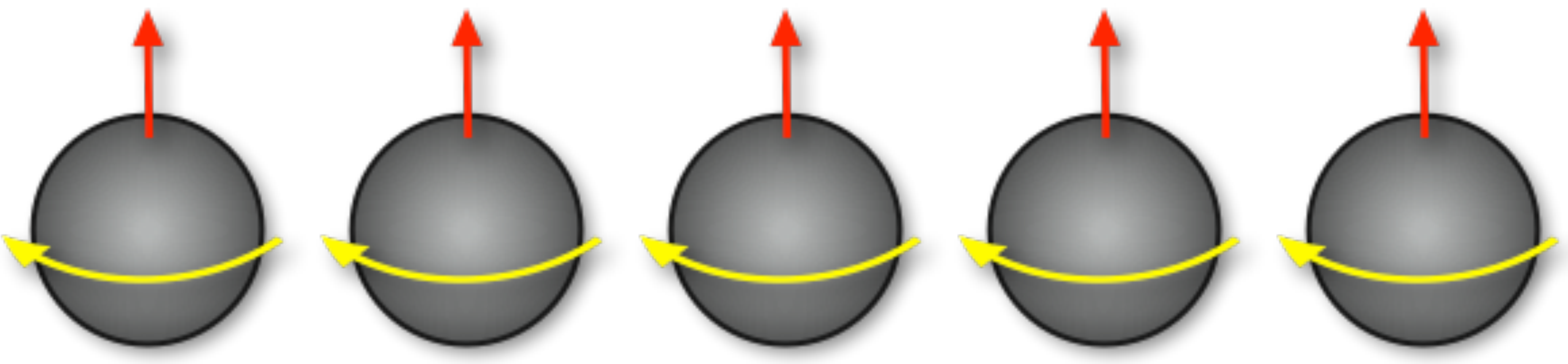
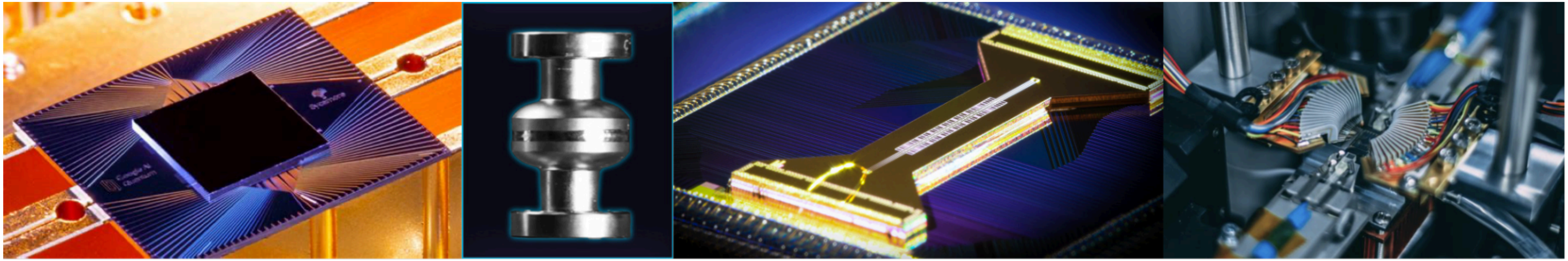
What is *quantum* computing?

- Quantum computing is using quantum systems to simulate our algorithms.
- Challenges are rooted in the fact that quantum systems are *delicate*. And algorithms are non-obvious.
- Multiple, “competing” platforms for quantum computation exist. The ultimate goals are *scale* and *quantum error correction*.

There are many ways to leverage quantum systems to simulate an algorithm. Features of quantum measurement mean the calculations are probabilistic.



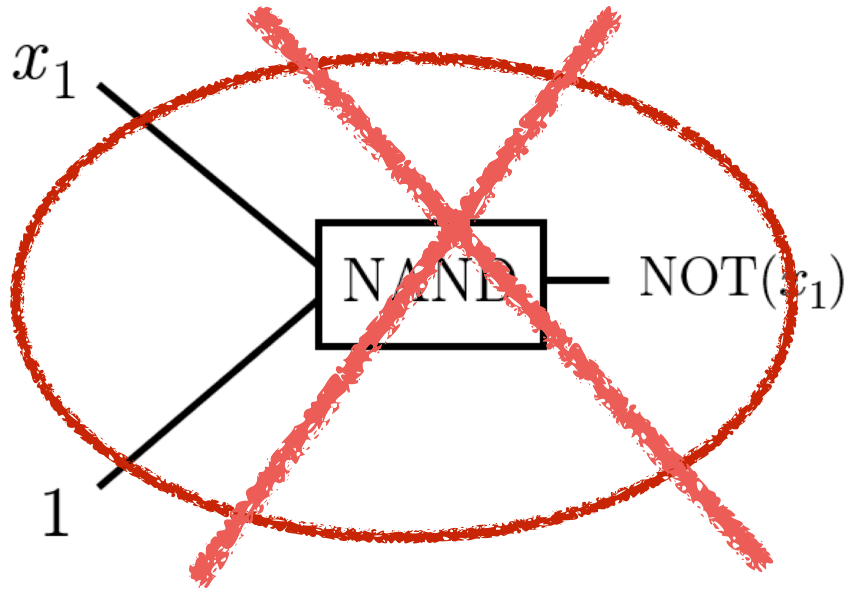


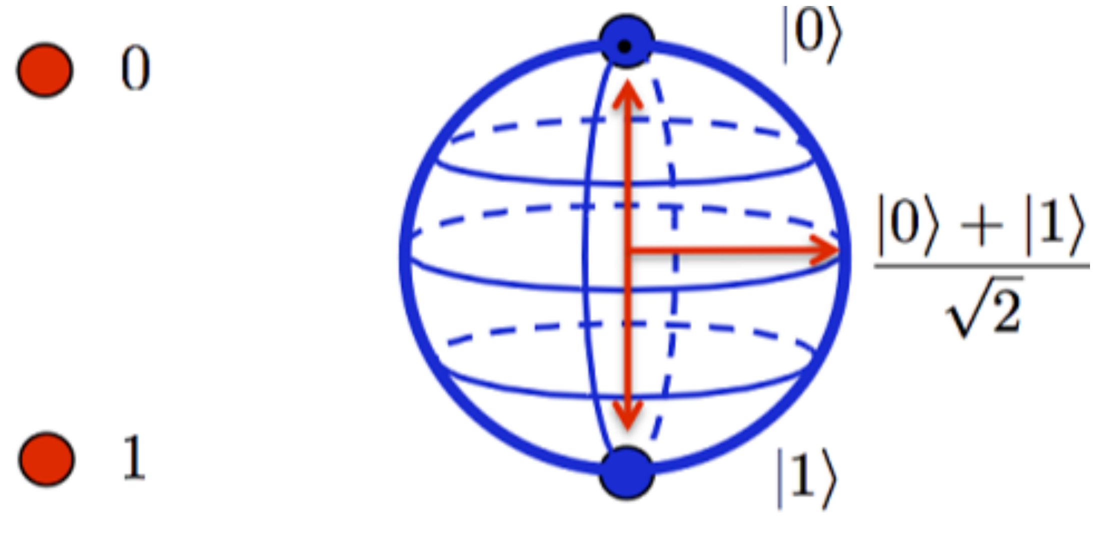
https://ai.googleblog.com/2019/10/quantum-supremacy-using-programmable.html
https://sqms.fnal.gov/research/

https://www.honeywell.com/en-us/company/quantum
https://www.xanadu.ai/hardware

What *is* quantum computing?

- At heart, quantum computing is unitary evolution of quantum states.
- It is distinguished by the following features:
  - Entanglement
  - Unitary evolution
  - Superposition of states
  - Reversible computation
  - Probabilistic computation
  - Exponential Hilbert spaces
  - Challenges with state coherence





Classical Bit **Qubit**

Quantum computing power* scales exponentially with qubits
N bits can exactly simulate log N qubits

This compute unit....	 Commodore 64	 AWS M4 Instance 1 Million x Commodore 64	 Entire Global Cloud 1 Billion x (1 Million x Commodore 64)
can exactly simulate:	**10 Qubits**	**30 Qubits**	**60 Qubits**

What *is* quantum computing?

https://bit.ly/38bidph

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

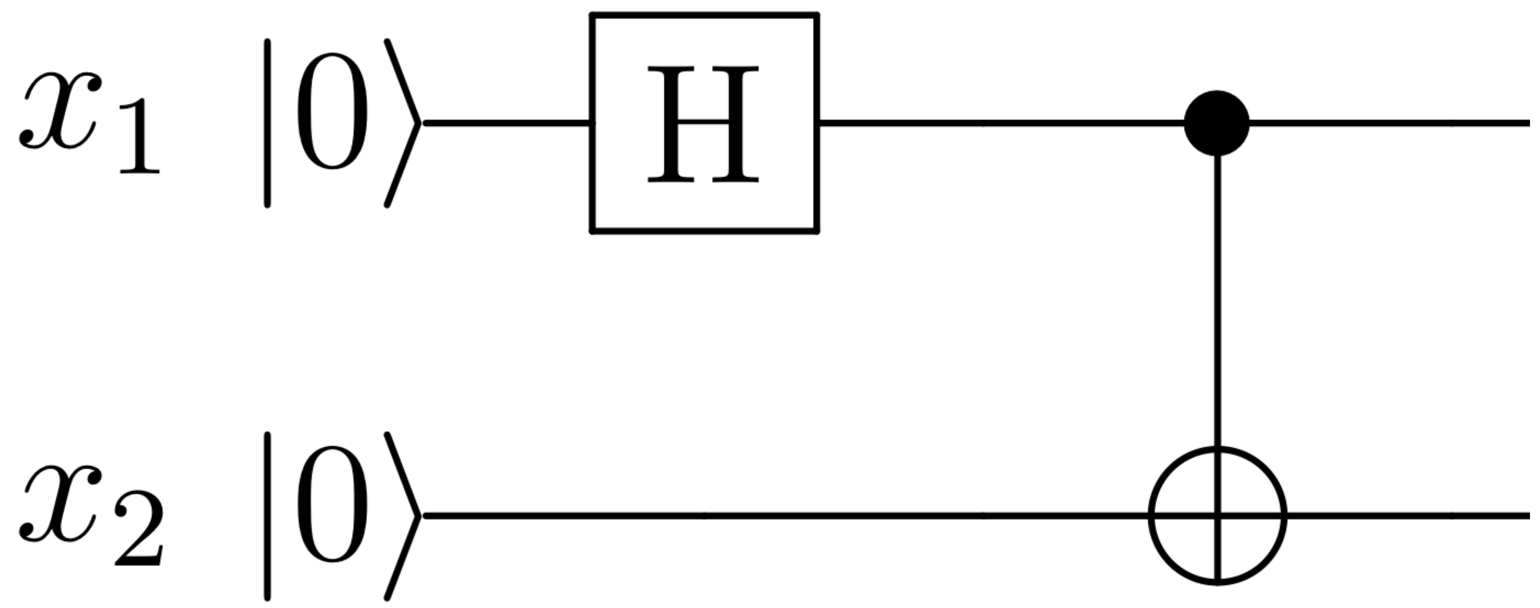
$$|0\rangle|0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix} 1\begin{pmatrix}1\\0\end{pmatrix} \\ 0\begin{pmatrix}1\\0\end{pmatrix}\end{pmatrix} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix} = |00\rangle$$

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

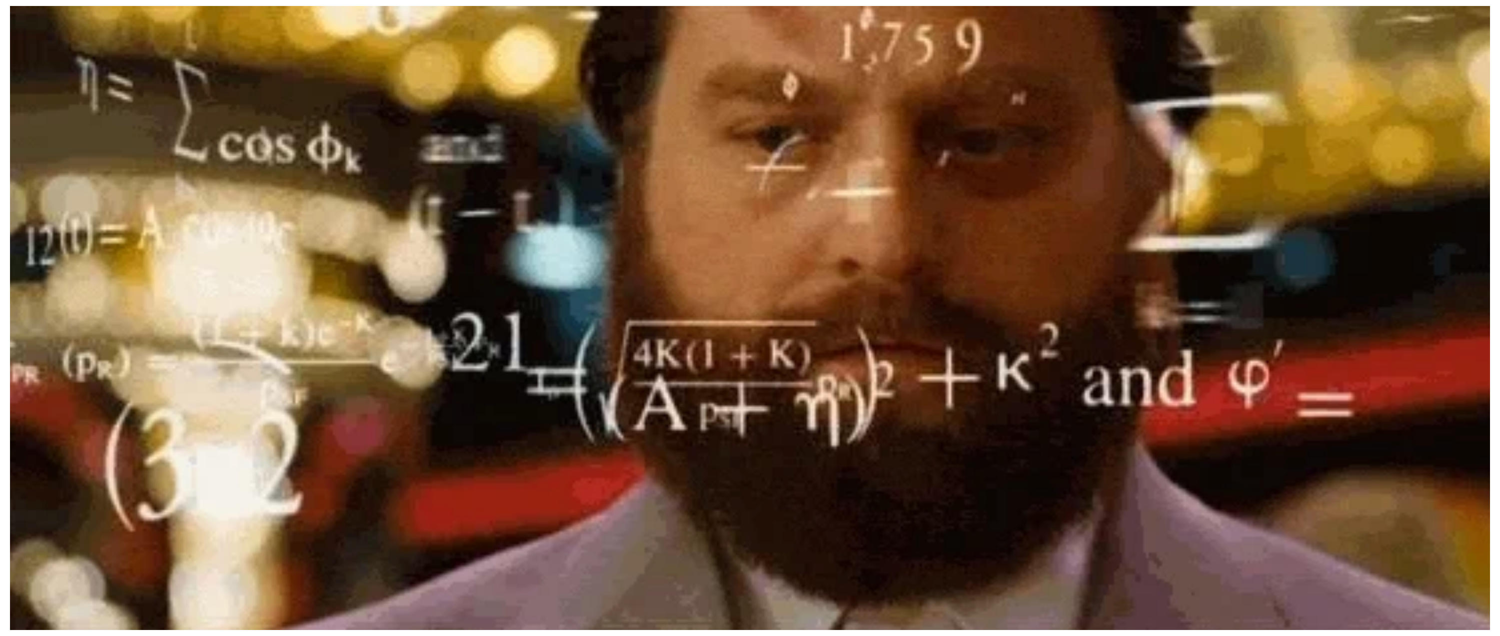
$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \equiv |+\rangle$$

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

Superposition!



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

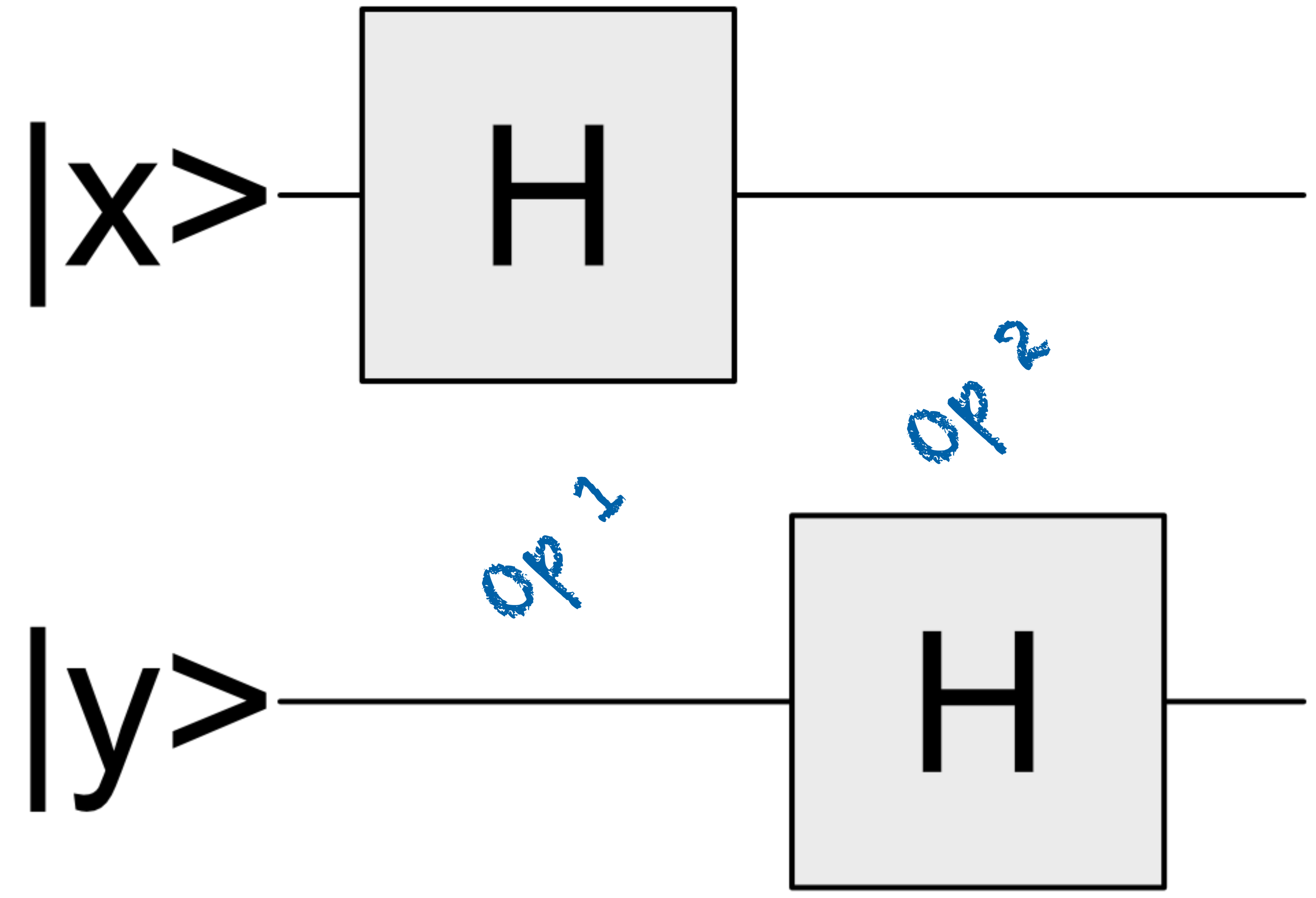


Entanglement!

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

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

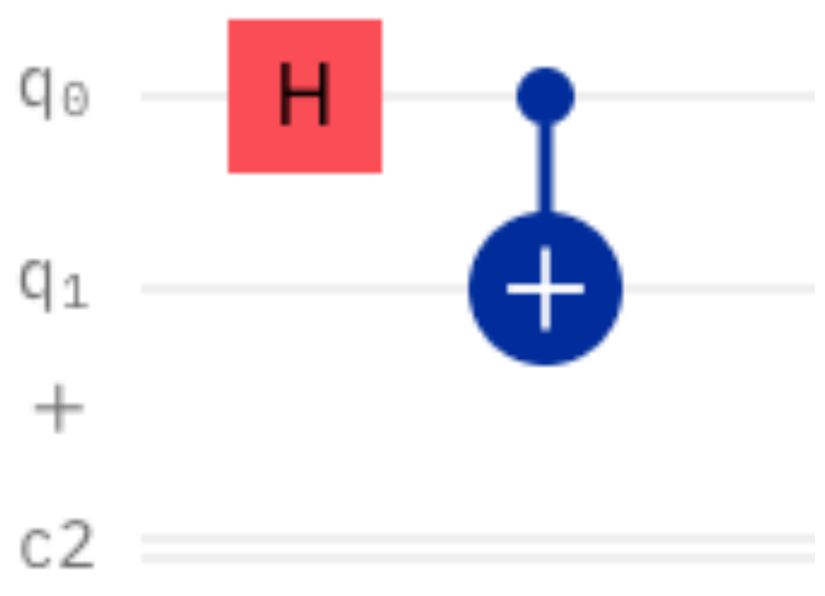
What *is* quantum computing?

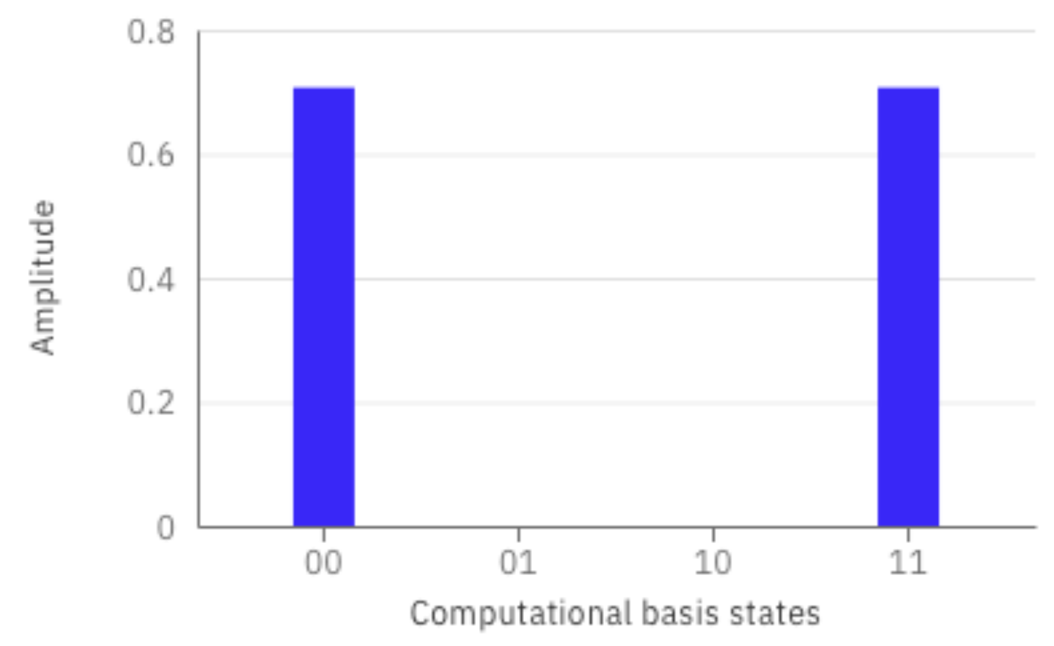


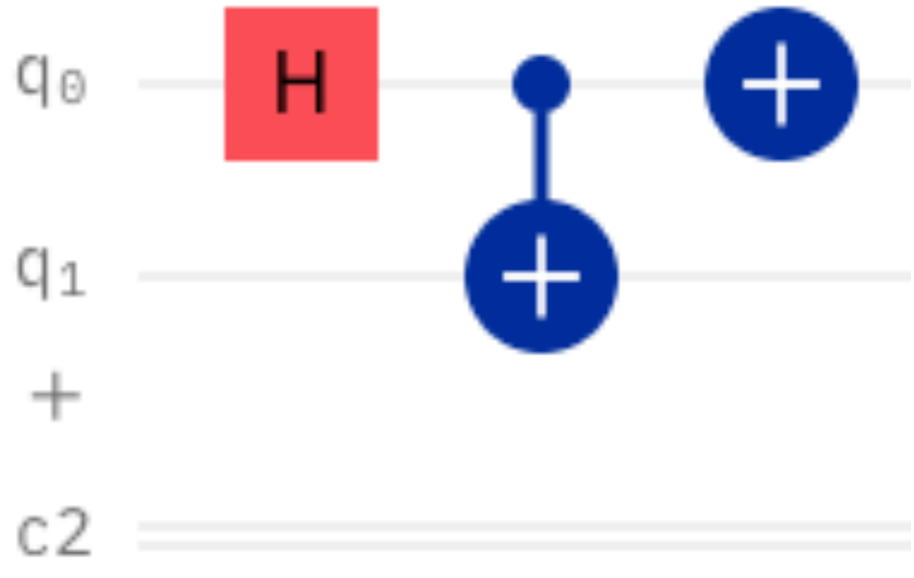
$$H \otimes I \qquad\qquad I \otimes H$$

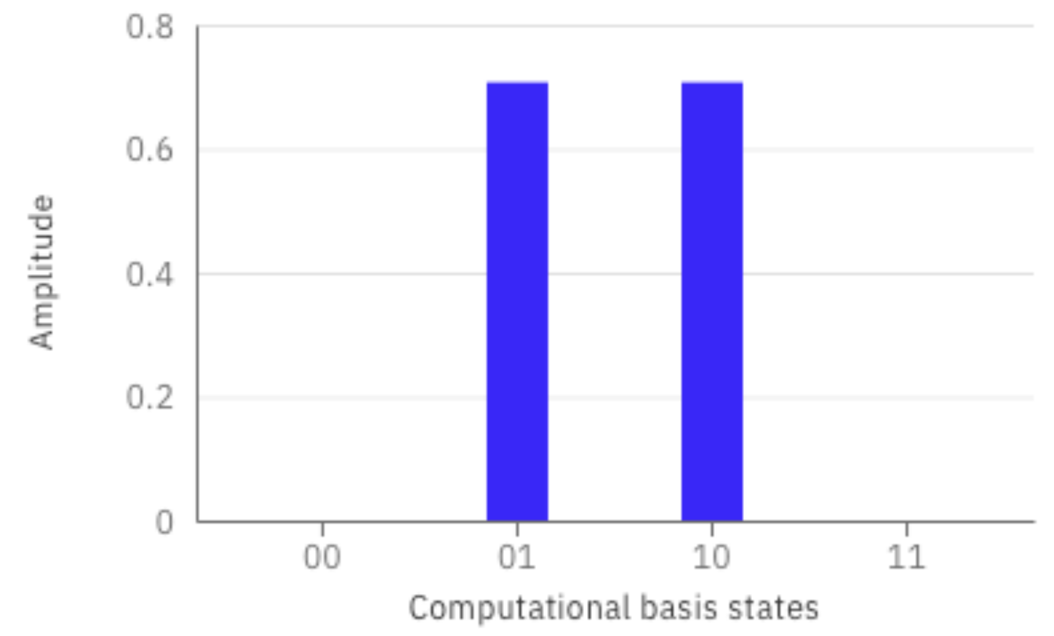
$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix}$$

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









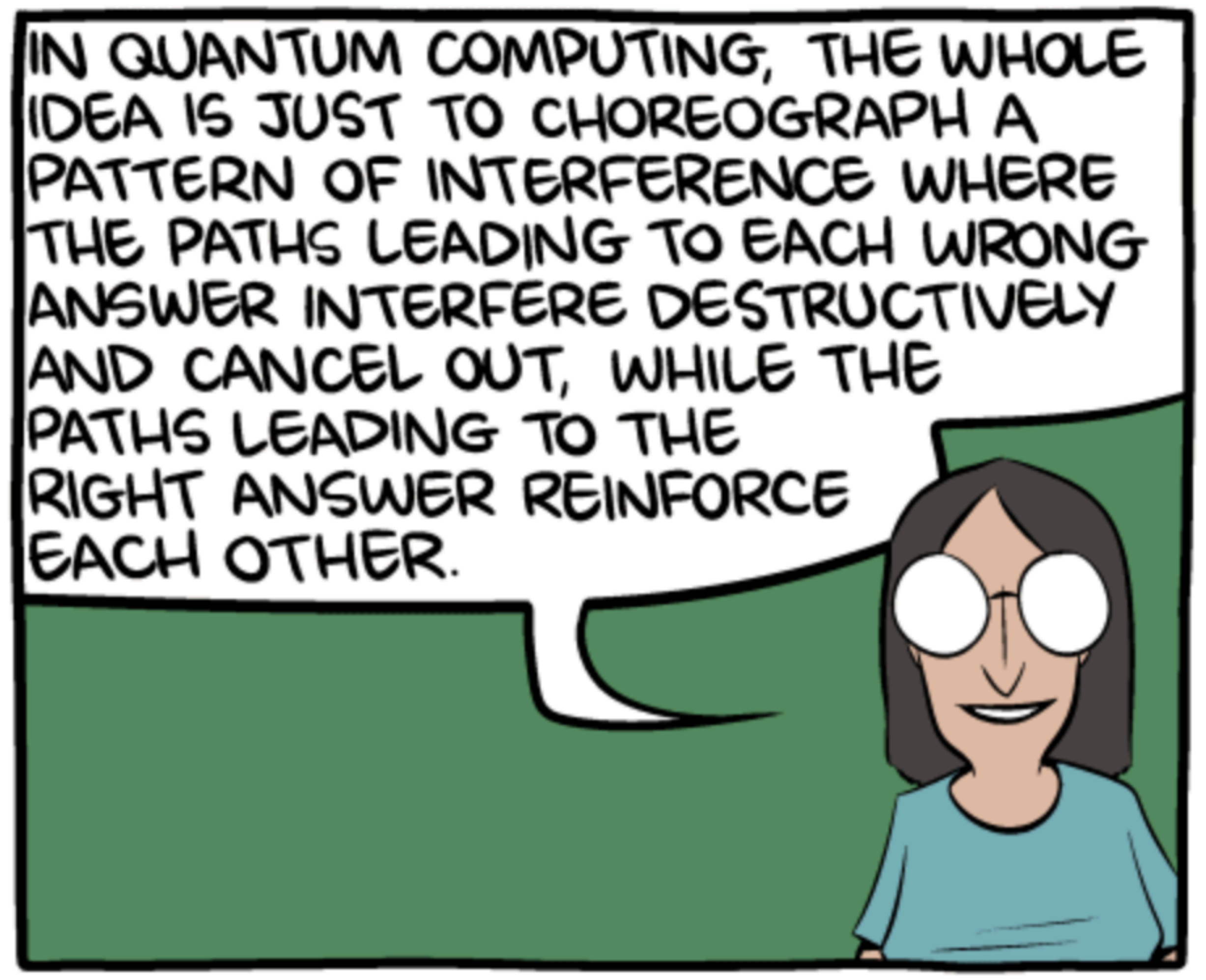
Super hand-wavy "quantum advantages"

- 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…)

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.

SQMS

SUPERCONDUCTING QUANTUM MATERIALS & SYSTEMS CENTER

https://sqms.fnal.gov

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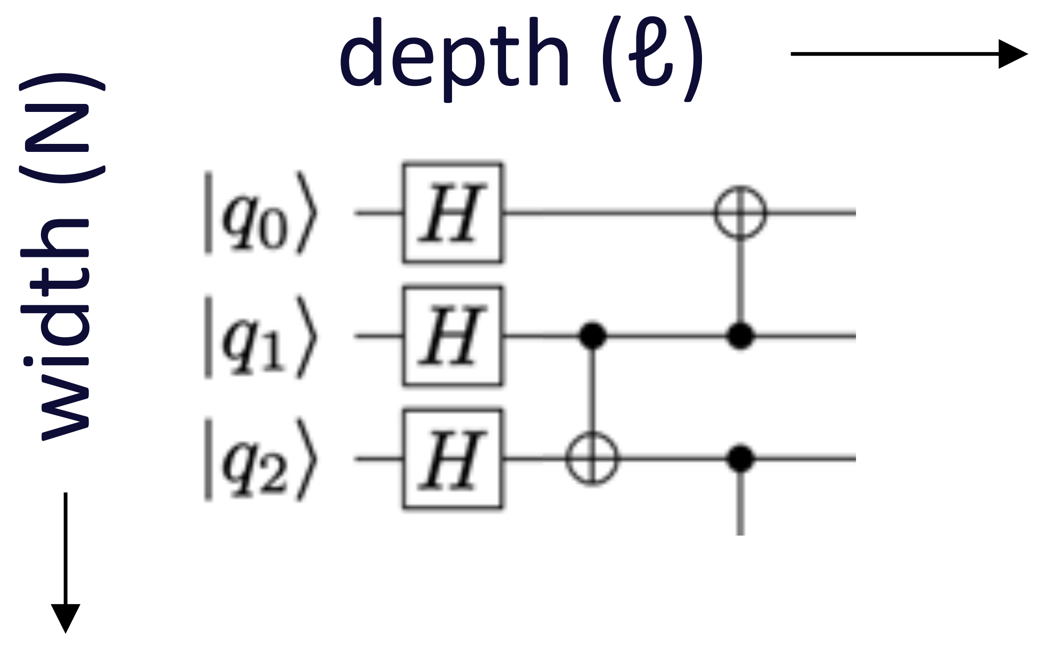
SQMS - mission

- ***The mission of the SQMS is to achieve transformational advances in the major cross-cutting challenge of understanding and eliminating the decoherence mechanisms in superconducting 2D and 3D devices, with the goal of enabling construction and deployment of superior quantum systems for computing and sensing.***
  - We will attack the coherence of scalable 2D devices with strengths in materials and low loss RF superconductivity, and the scalability of record coherence 3D devices with strengths in large high Q RF cry-systems integration.
  - In quantum computing we will build alpha prototypes of 2D and 3D quantum information processors with revolutionary capabilities.
  - In quantum sensing we will purse fundamental physics questions by leveraging SRF cavity-based quantum technologies.
    - *WE ARE FIRST AND FOREMOST ABOUT BUILDING STUFF!*

SQMS Will Reach New Limits of Coherence for Superconducting Qubits

Quantum algorithms:



Ultimate limits to depth:

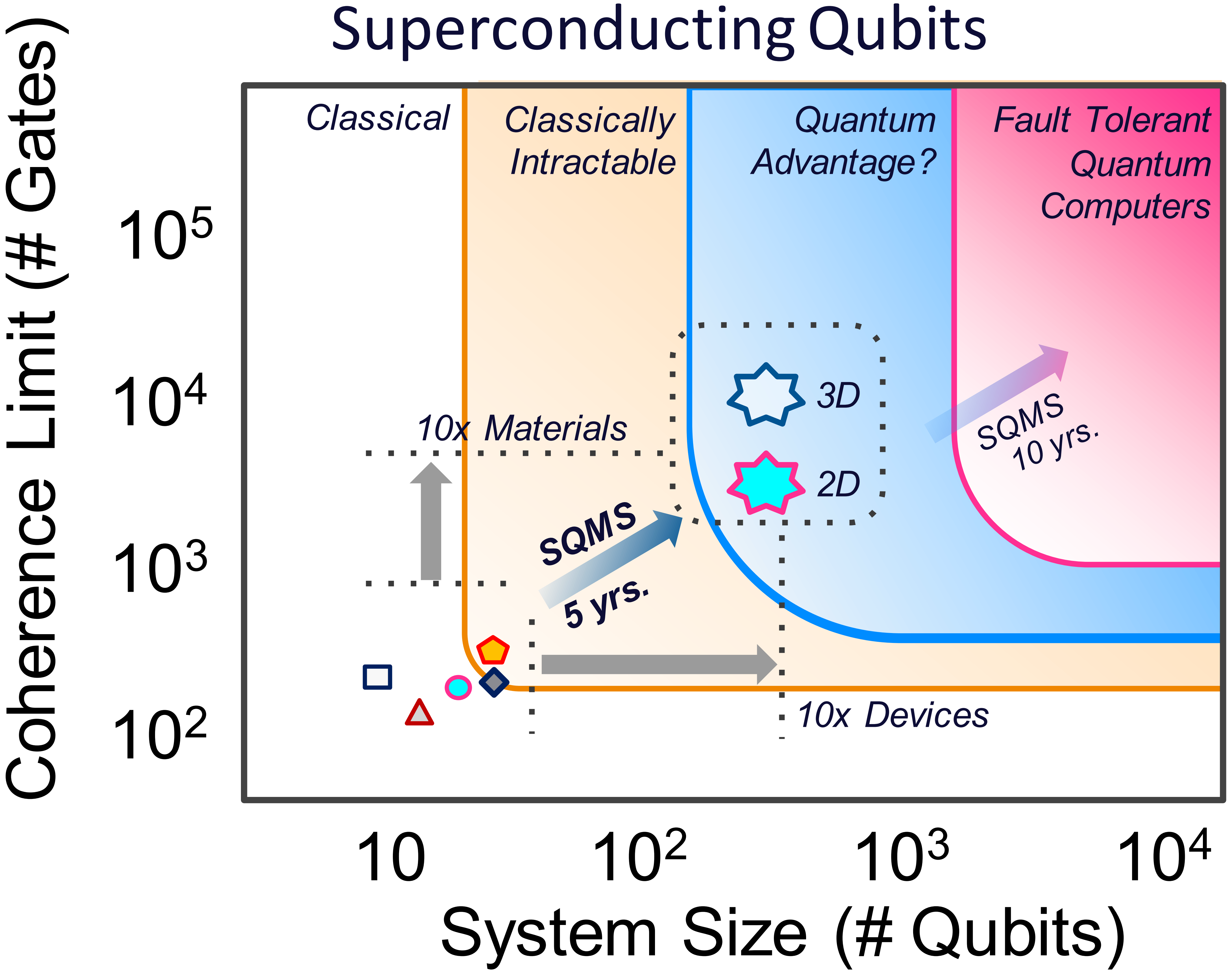
$\max(\ell) \propto T_1 / t_{gate}$

For SC qubits, typical:

t_{gate} = [20-1000] ns

$\max(N^*\ell) \sim 10^4$

Superconducting Qubits



SQMS Consequences:

- SQMS-3D
- SQMS-2D

Leading US testbeds:

- *Google Sycamore*
- *IBM Hexagonal*
- *Rigetti Aspen*
- *Yale Single-mode*
- *UChicago Multi-mode*

Slide by Chad Rigetti, CEO Rigetti Computing

SQMS member institutions

- DOE laboratories + Industry leaders + Academia
- Extraordinary portfolio of knowledge, skills, and facilities deployed to tackle the physics of decoherence and to build and deploy a revolutionary quantum information platform for sensing and computation.

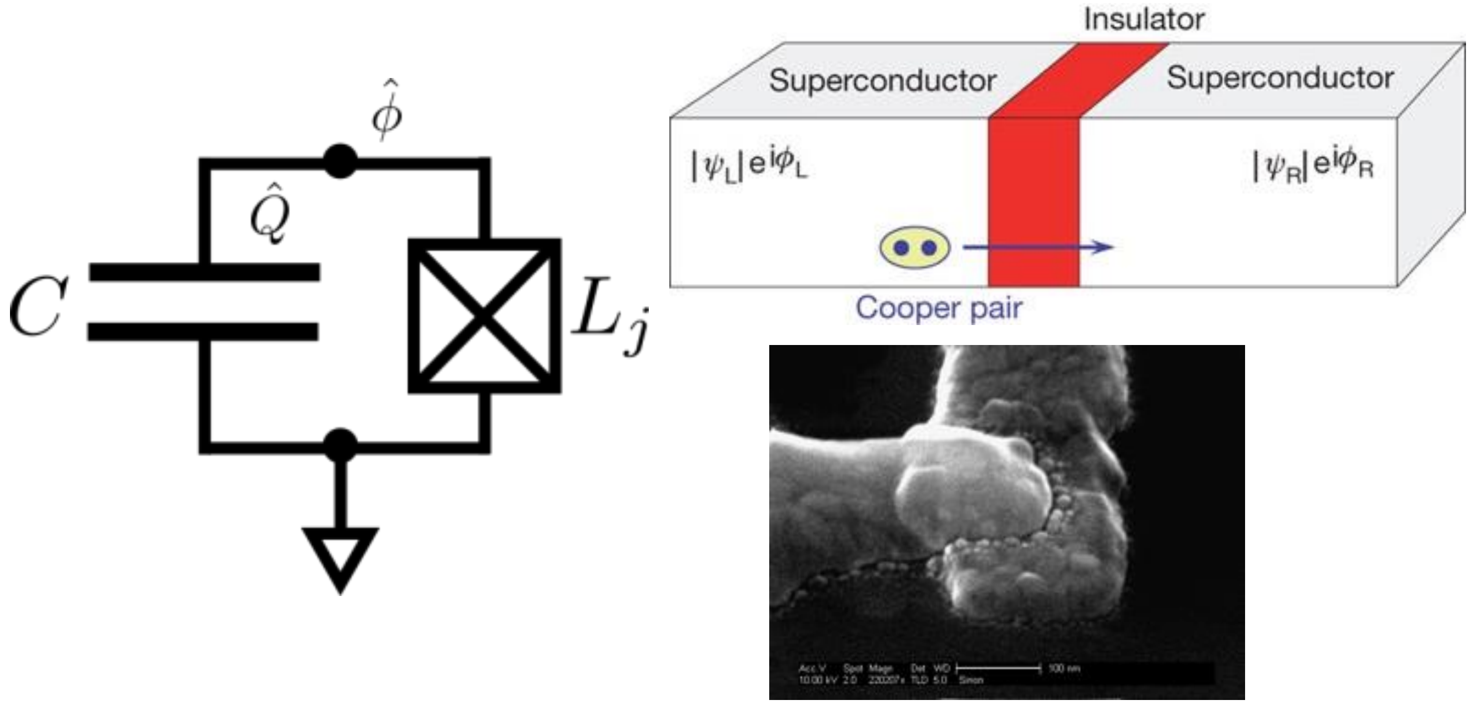
Slide material courtesy of Anna Grassellino (FNAL)

Slide material courtesy of
Anna Grassellino (FNAL)

2D and 3D quantum devices

- Our qubits use superconducting technologies - coherence is a critical feature!
- SQMS Jargon
  - "2D": arrays of superconducting transmons (mostly built by Rigetti Computing)
  - "3D": superconducting transmons coupled to a resonator cavity (particularly SRF cavities)

1. LC circuit with Josephson junction



"Transmon" qubits

J. Koch et al, Phys. Rev. **A** 76, 042319 (2007)

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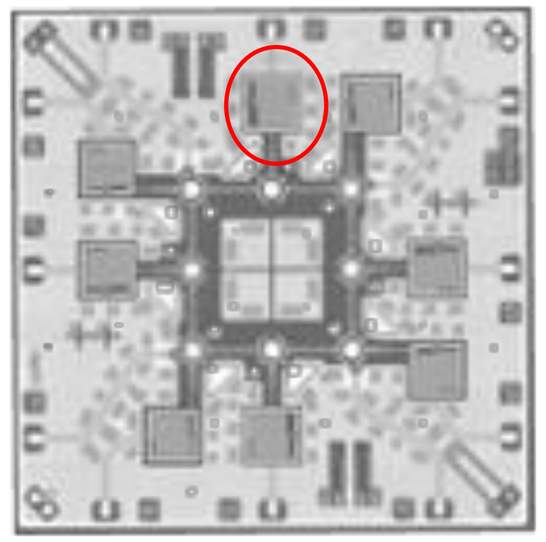
2. Resonators (cavities)

2D



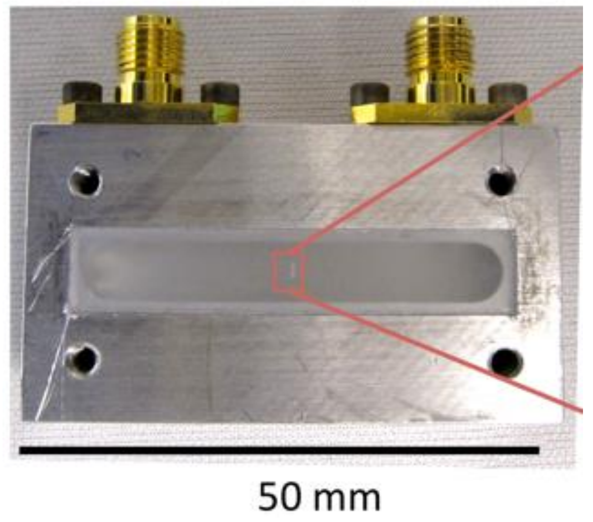
Rigetti 8-qubit processor

Q ~ 10^5

$T_{coherence}$ ~ 0.000001 s

M. Reagor et al, Science Advances, Vol.4, no. 2, (2018)

3D



3D transmon

Q ~ 10^8

$T_{coherence}$ ~ 0.001 s

H. Paik et al, Phys. Rev. Lett. 107, 240501 (2011)

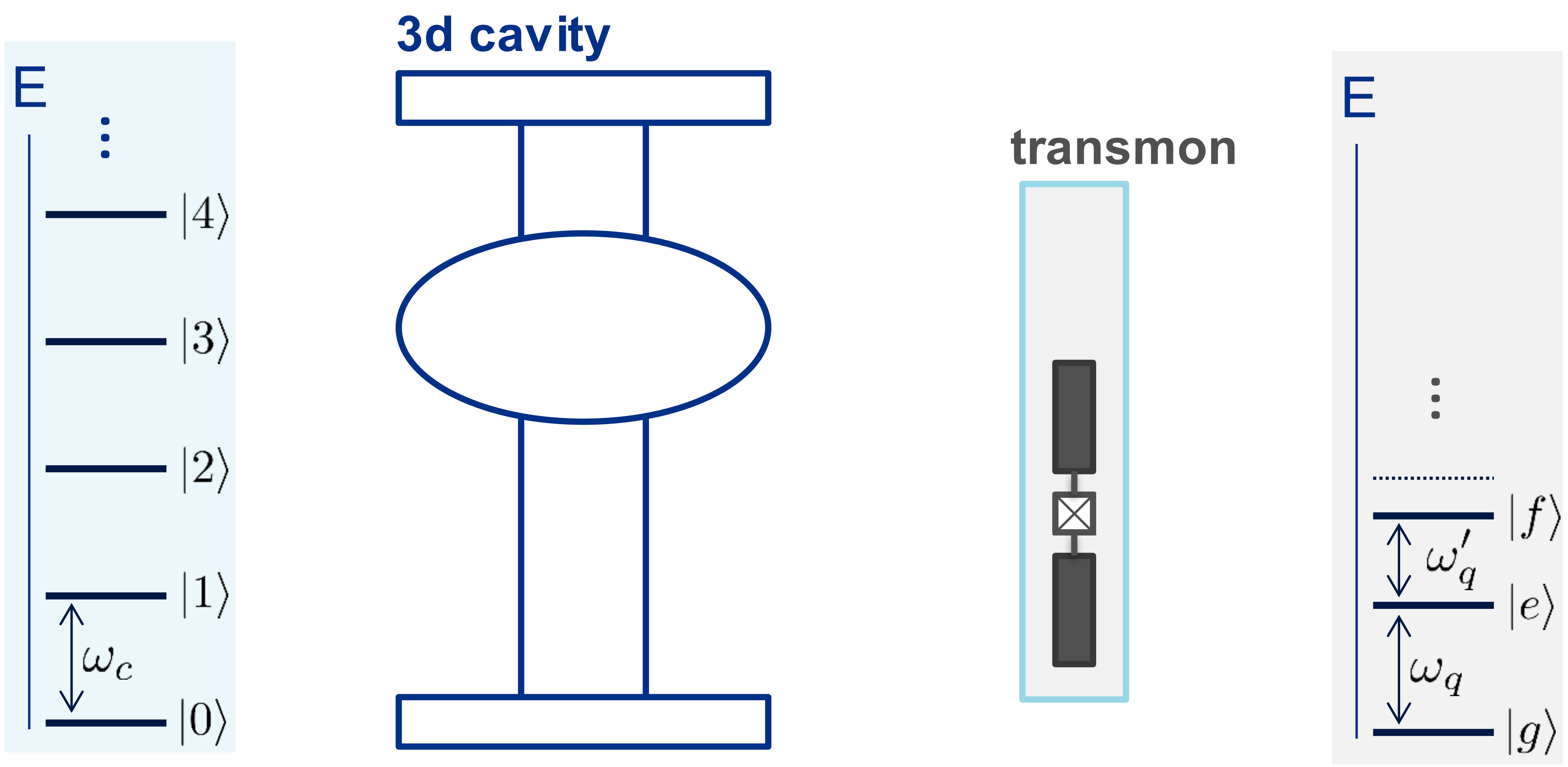
Fermilab SRF resonators

Q > 10^{10}

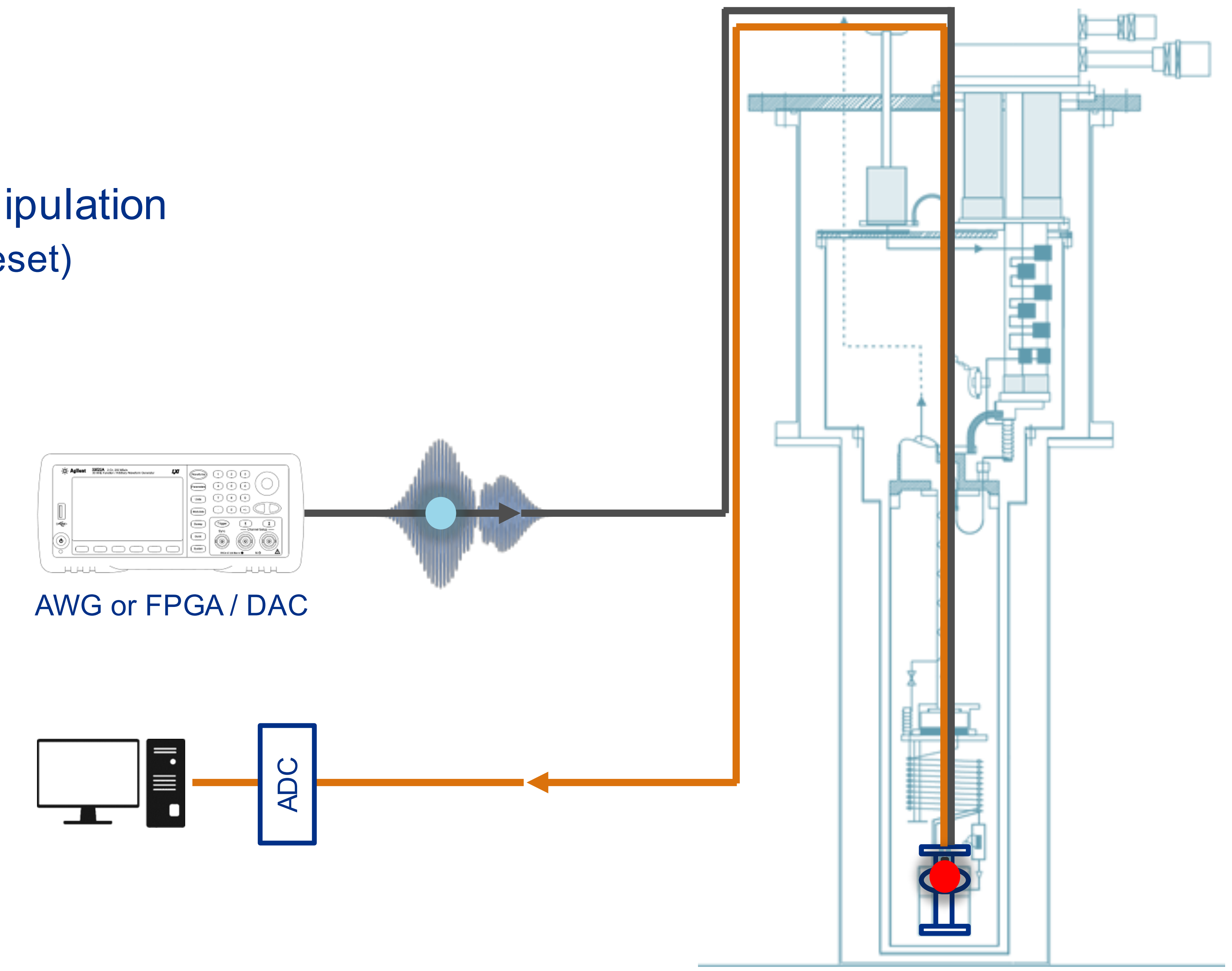
$T_{coherence}$ > 1 s

A. Romanenko et al, Phys. Rev. Appl. 13, 134052 (2020)

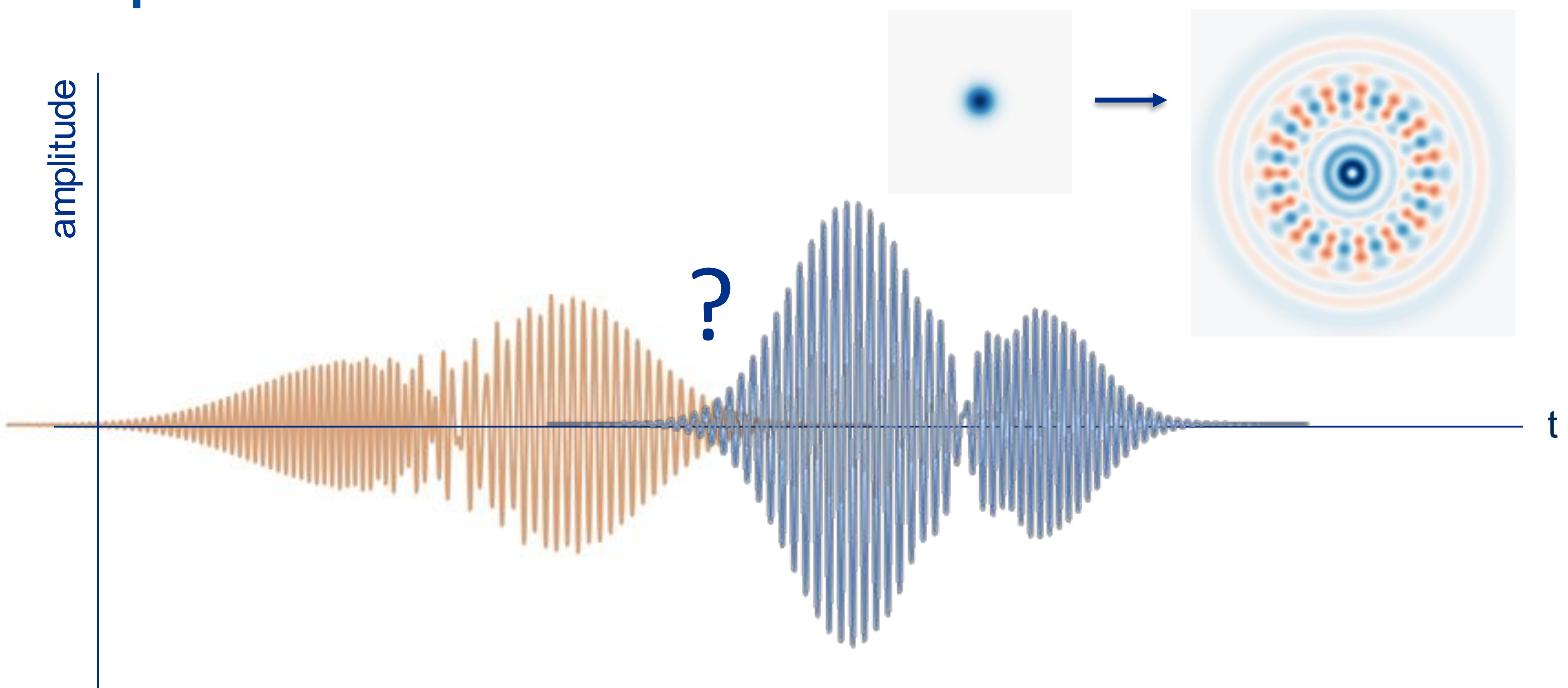
3d QPU: building blocks



1. Quantum state manipulation
   (unitary gates, fast reset)
2. Readout

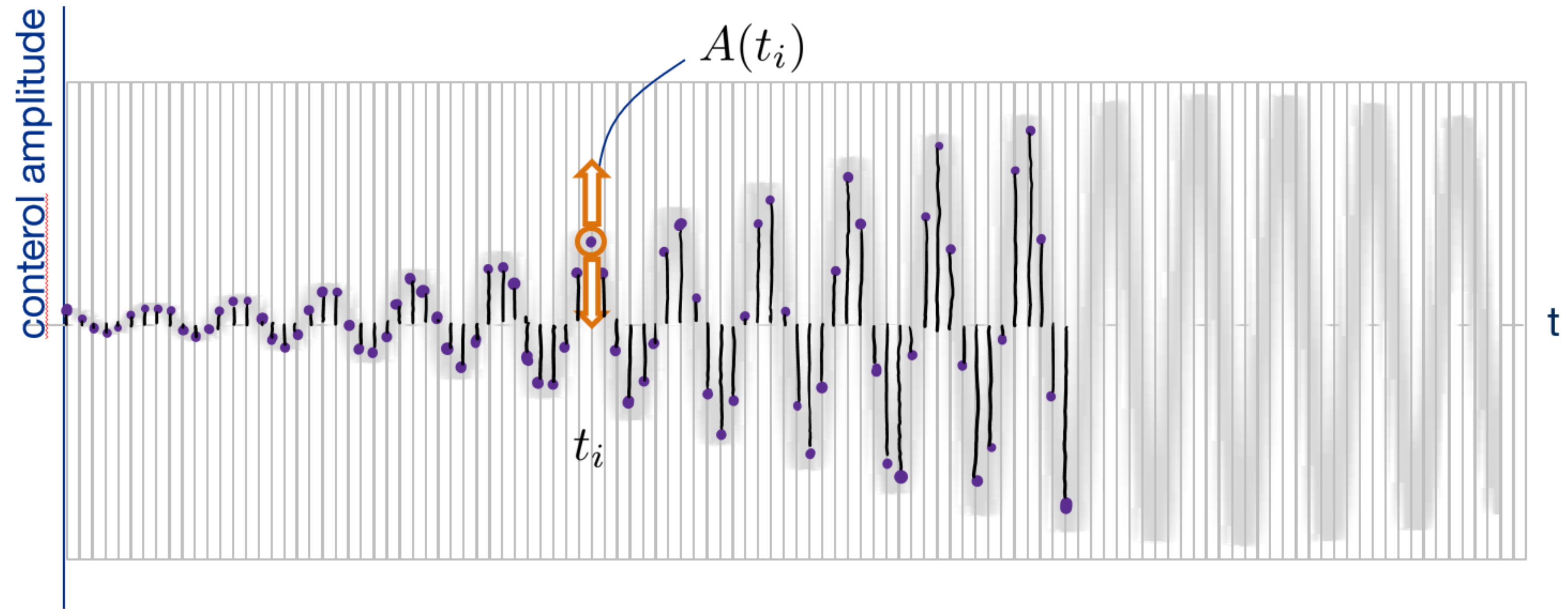


Control pulses



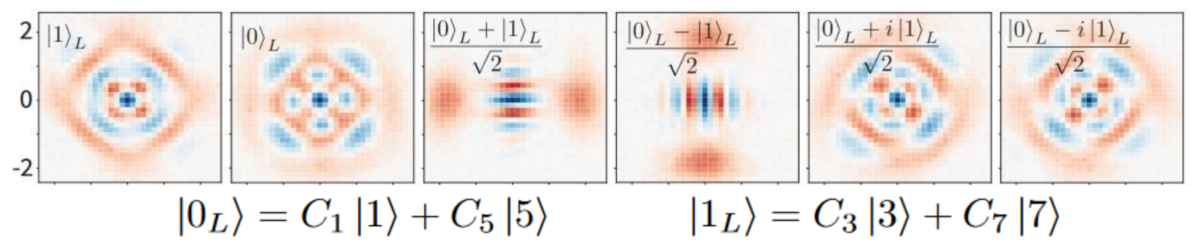
Slide material by Jens Koch, Northwestern

Optimal control theory:



find:

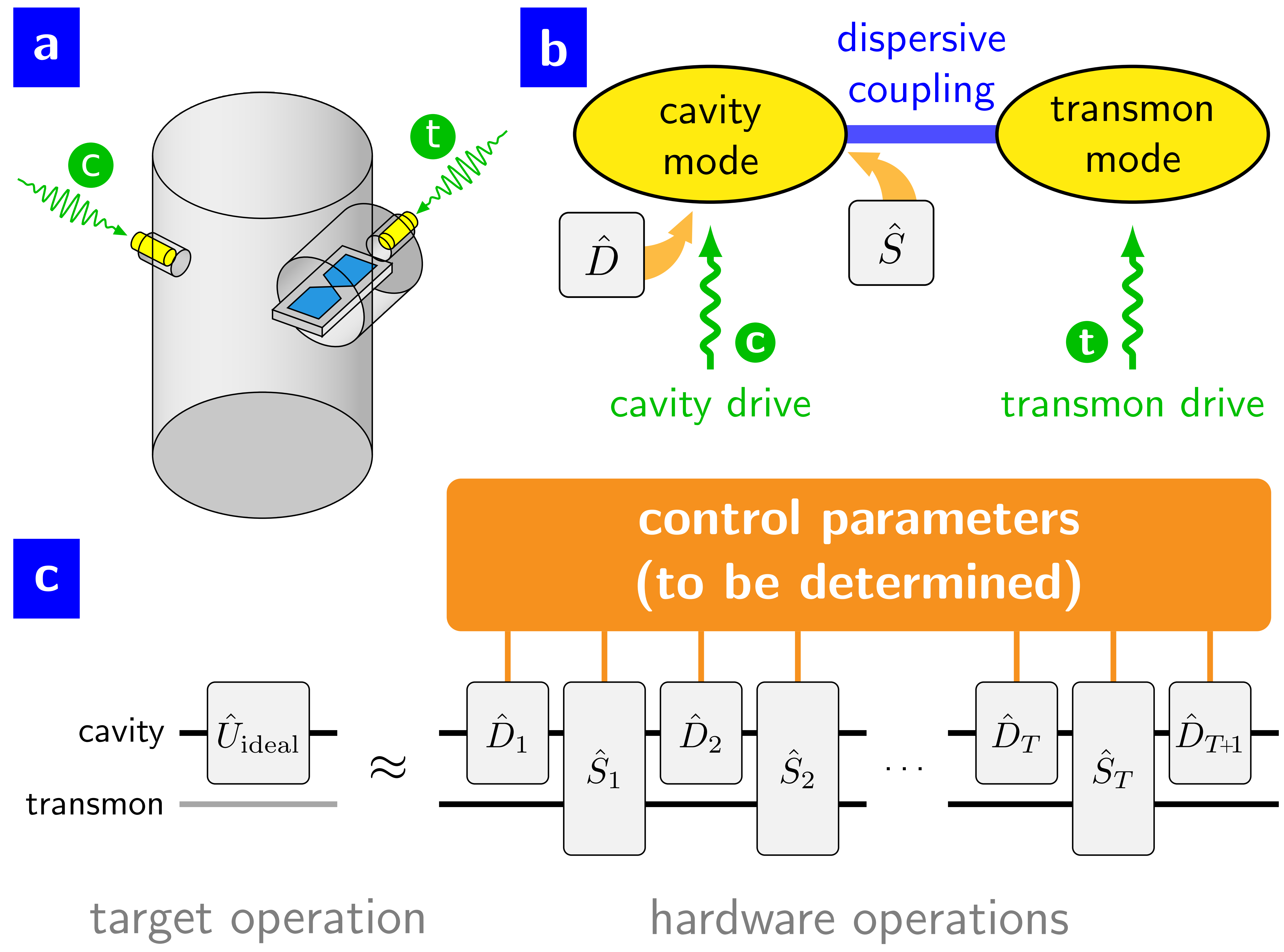
$$\max \mathcal{F}[A(t)]$$



success story:

Autonomous error correction of cavity based qubit
J. Gertler et al., arXiv:2004.09322 (2020)

Controlling 3D quantum devices



T. Fosel et al, https://arxiv.org/abs/2004.14256

- One approach*:
  - Transmon qubit is coupled to the cavity.
  - Cavity drives and modes - cavity modes store quantum information.
  - Cavity drive allows cavity displacements.
  - Dispersive coupling allows the transmon drive to implement Selective Number-dependent Arbitrary Phase (SNAP) gates.
  - SNAPs and displacements form a **universal** set for quantum computing.

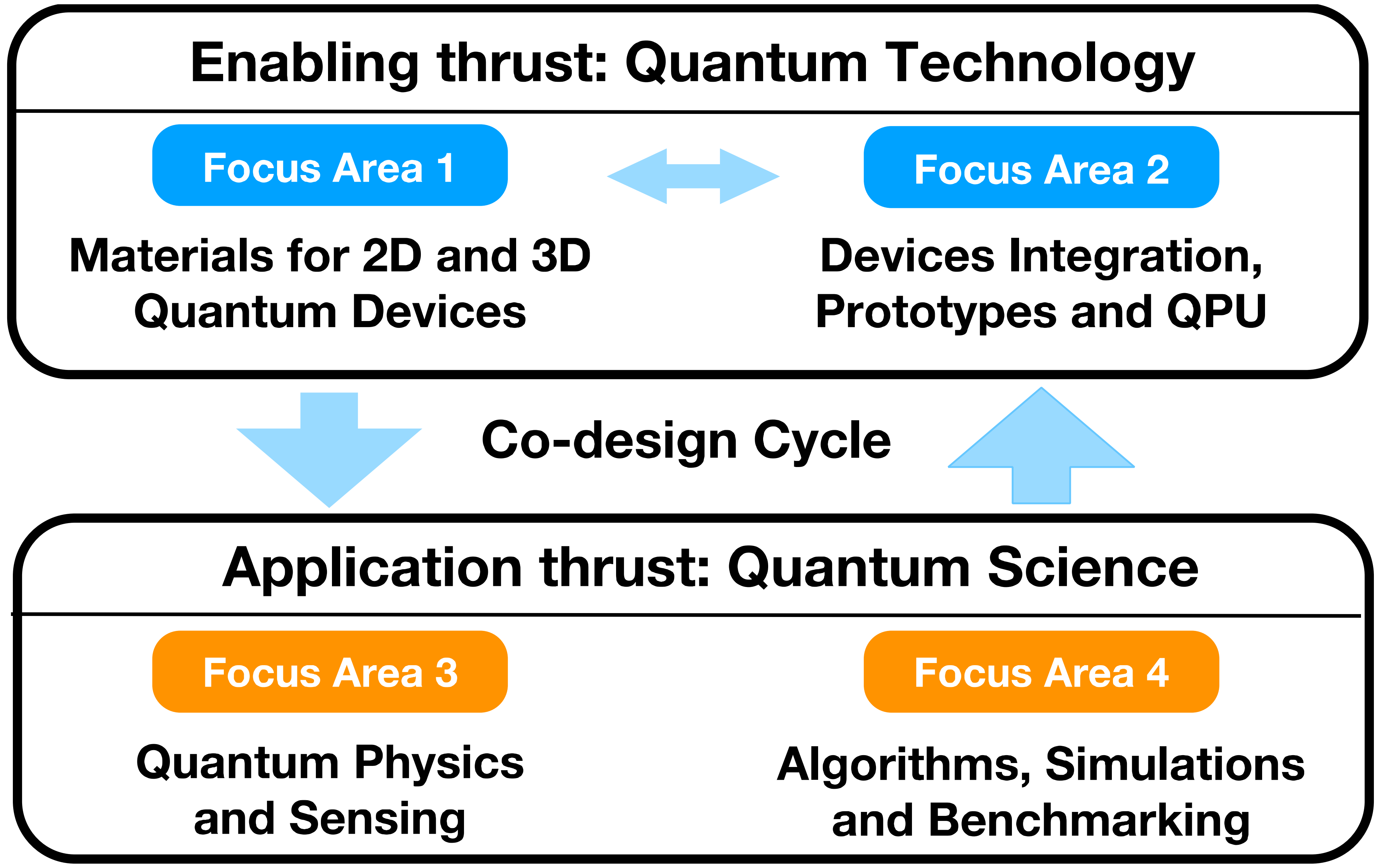
S. Krastonov et al, Physical Review A, 92(4):040303, 2015.

*See also, e.g. C-H Wang et al, https://arxiv.org/abs/2009.07855

SQMS focus areas - *thrusts*

- Focus areas are organized around two primary *thrusts:*
  - Quantum Technology: materials and device research aimed at a revolutionary leap in quantum coherence; integration into 2D and 3D architectures, and
  - Quantum Science: new physics searches and new algorithms and simulations enabled by our new quantum information processors.
    - Highly focused - fundamental materials and device research enables an advanced quantum information platform that we will use for physics experiments and computing.

Each thrust, in turn, has two *focus areas.*



All the focus areas interact coherently.

Slide material courtesy of Anna Grassellino (FNAL)

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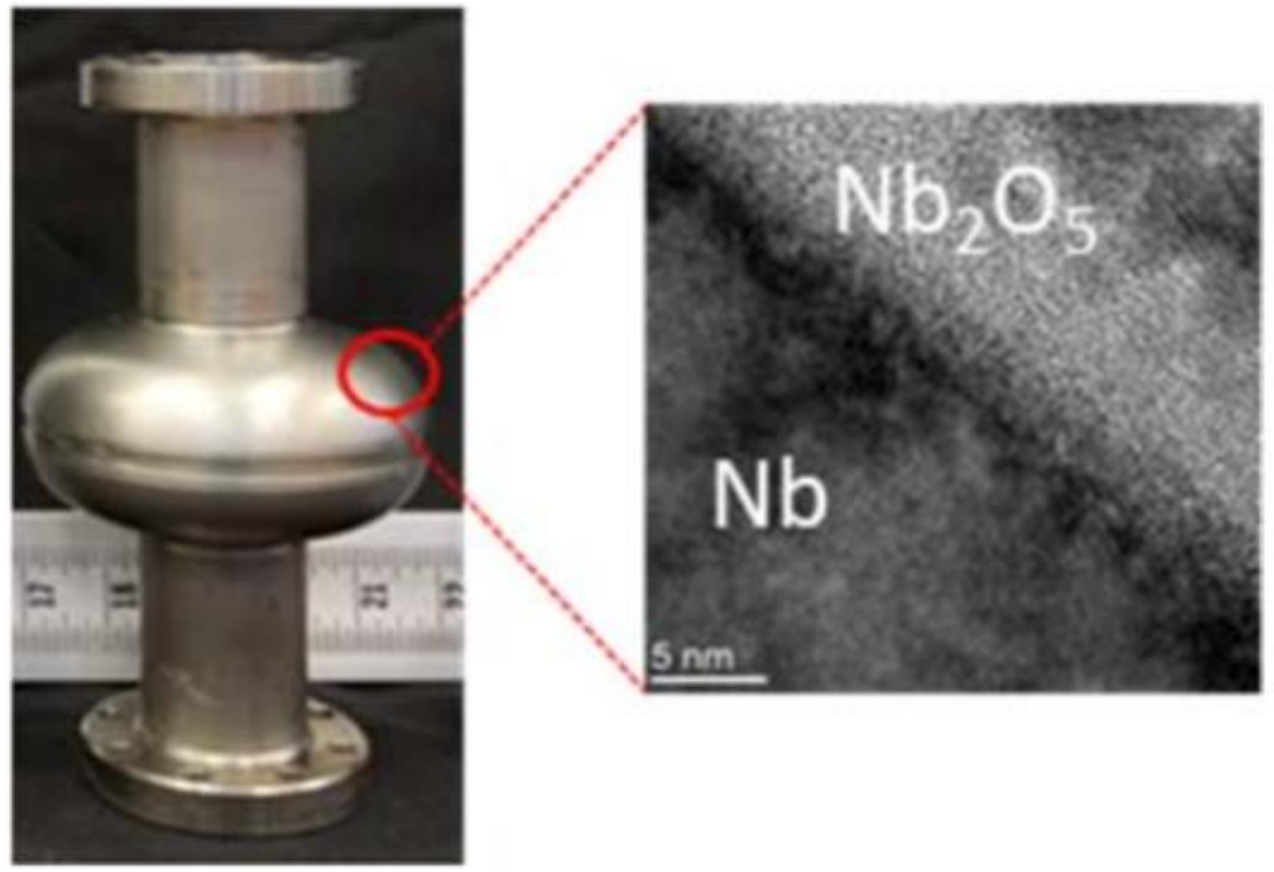
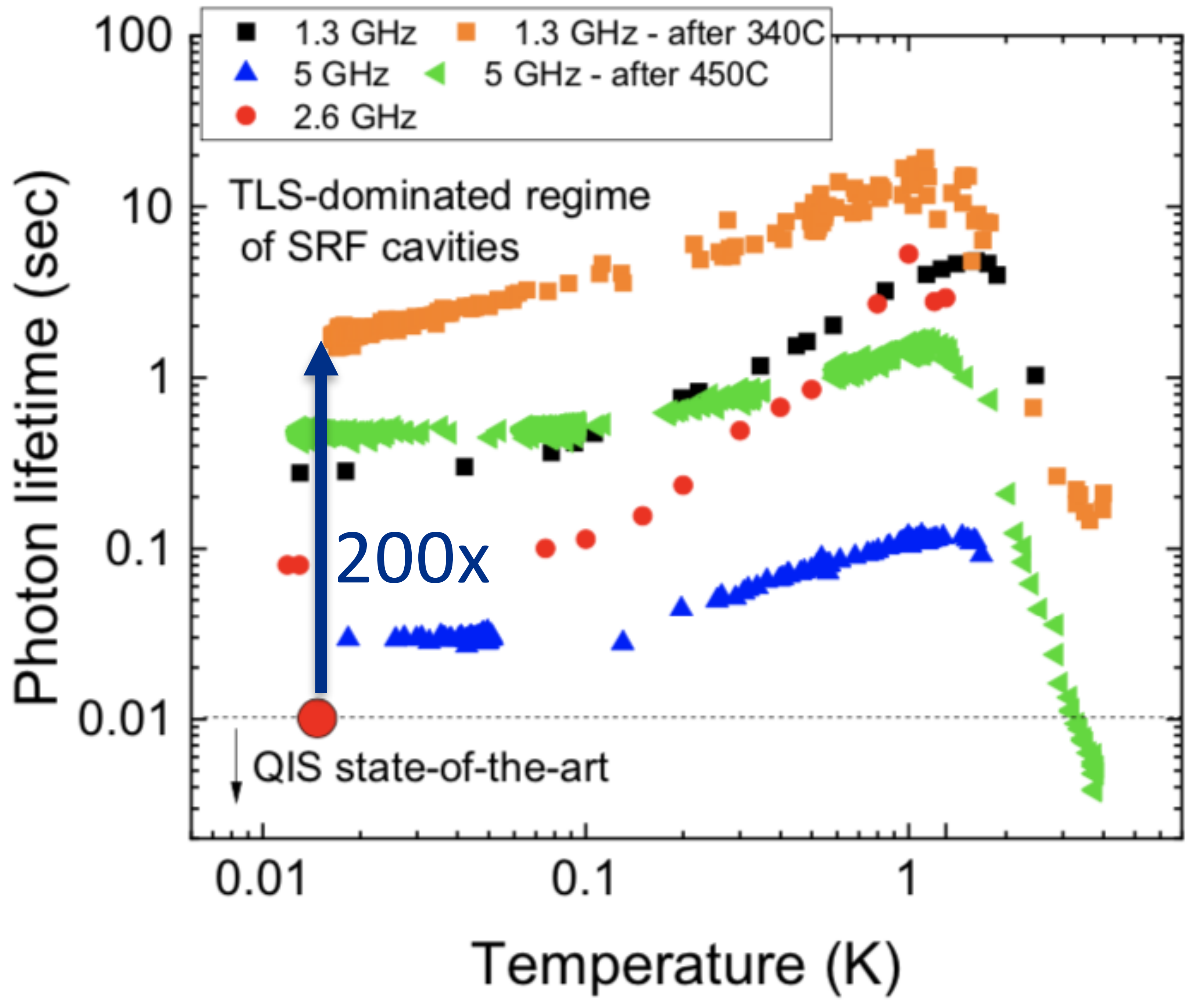
SQMS focus areas - focus area 1

Materials for 2D and 3D quantum devices

- Fermilab SRF resonators in the quantum regime for 3D architectures
  - Highest coherence quantum resonators ever demonstrated.
  - Achieved by combining device fabrication and testing with materials analysis: develop a more advanced understanding of device physics and performance.
  - Provides a large head start for further SQMS technology development.





A. Romanenko *et al*, Phys. Rev. Applied 13, 034032 (2020)

Slide material courtesy of Anna Grassellino (FNAL)

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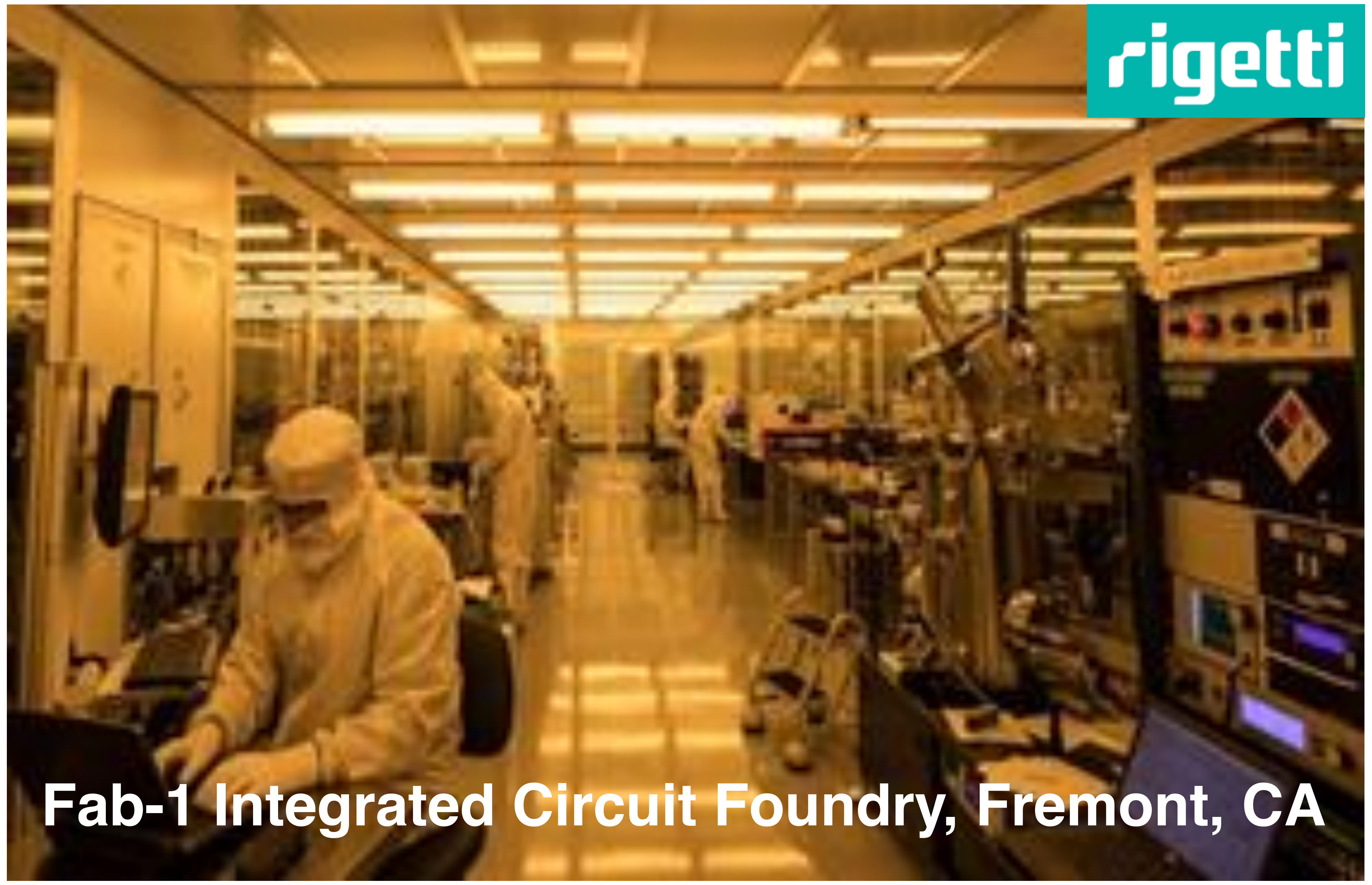
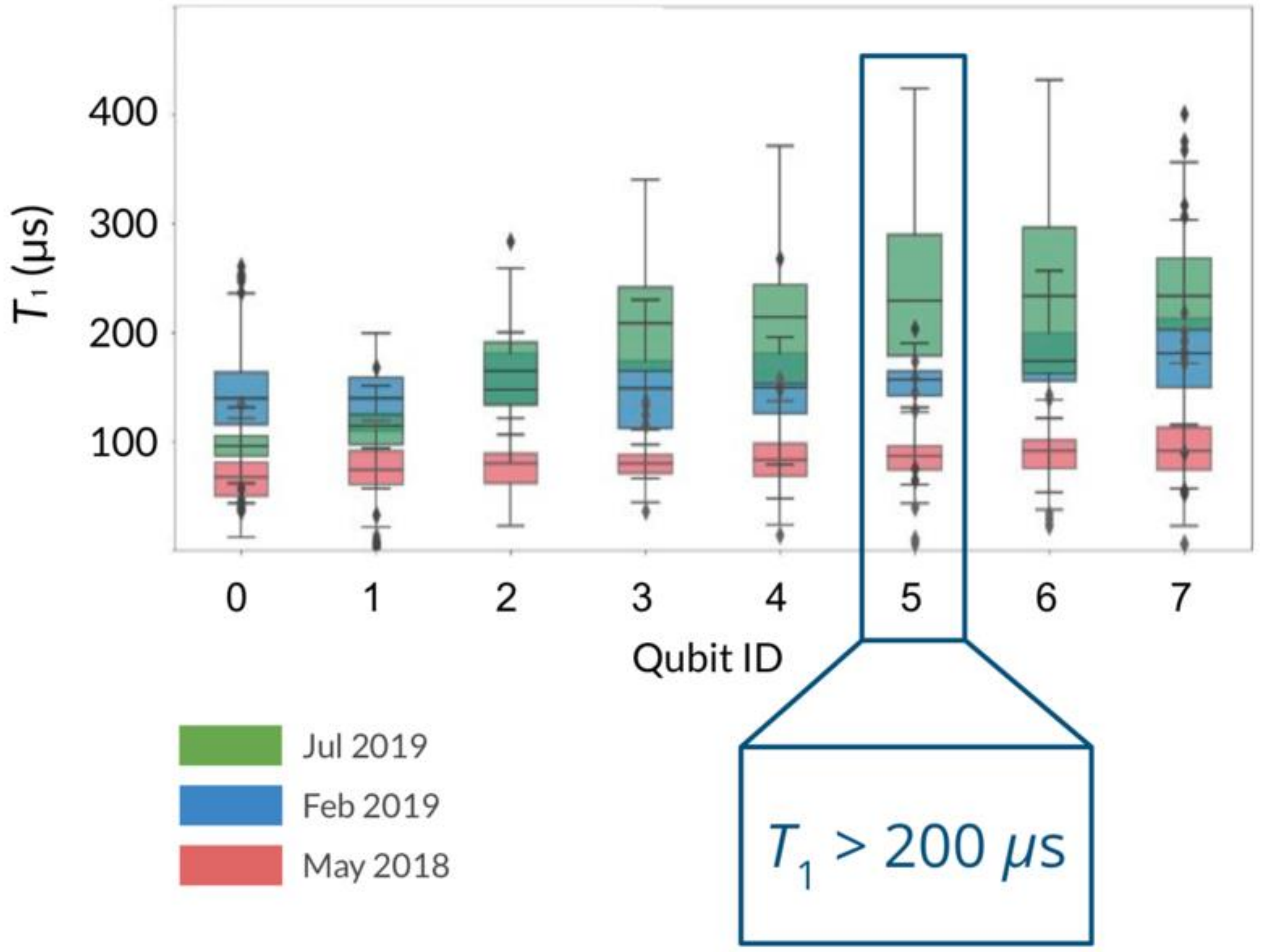
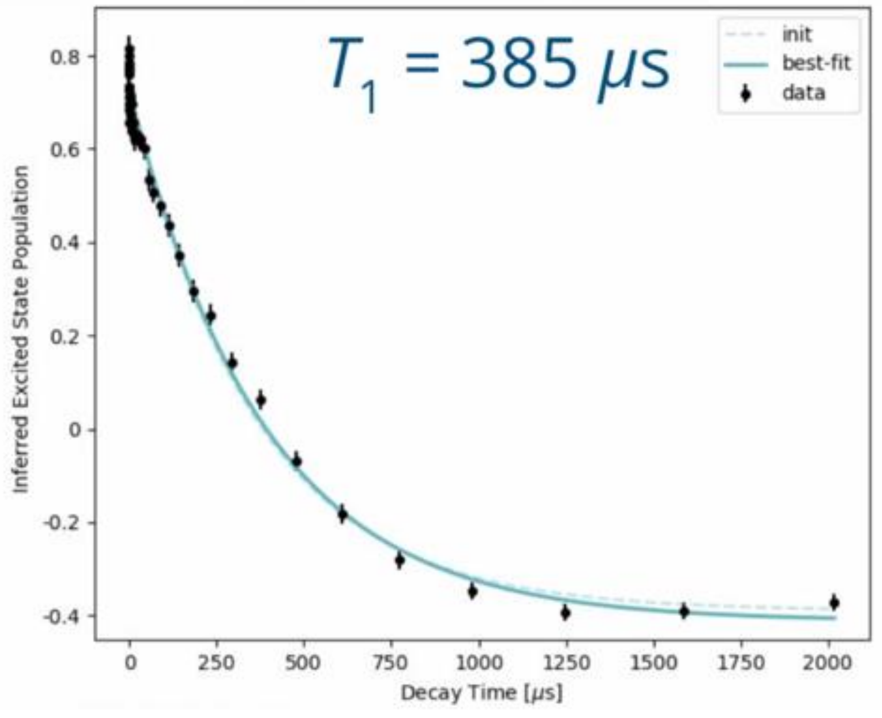
SQMS focus areas - focus area 1

Materials for 2D and 3D quantum devices

- To advance 2D architectures, we plan to leverage Rigetti's position at the forefront of qubit coherence and study hundreds of devices with material and surface science techniques to understand the origins of decoherence and the reasons underpinning device variability.
- This is enabled by the unique DOE BES and other material science facilities addition to planned investments and upgrades.







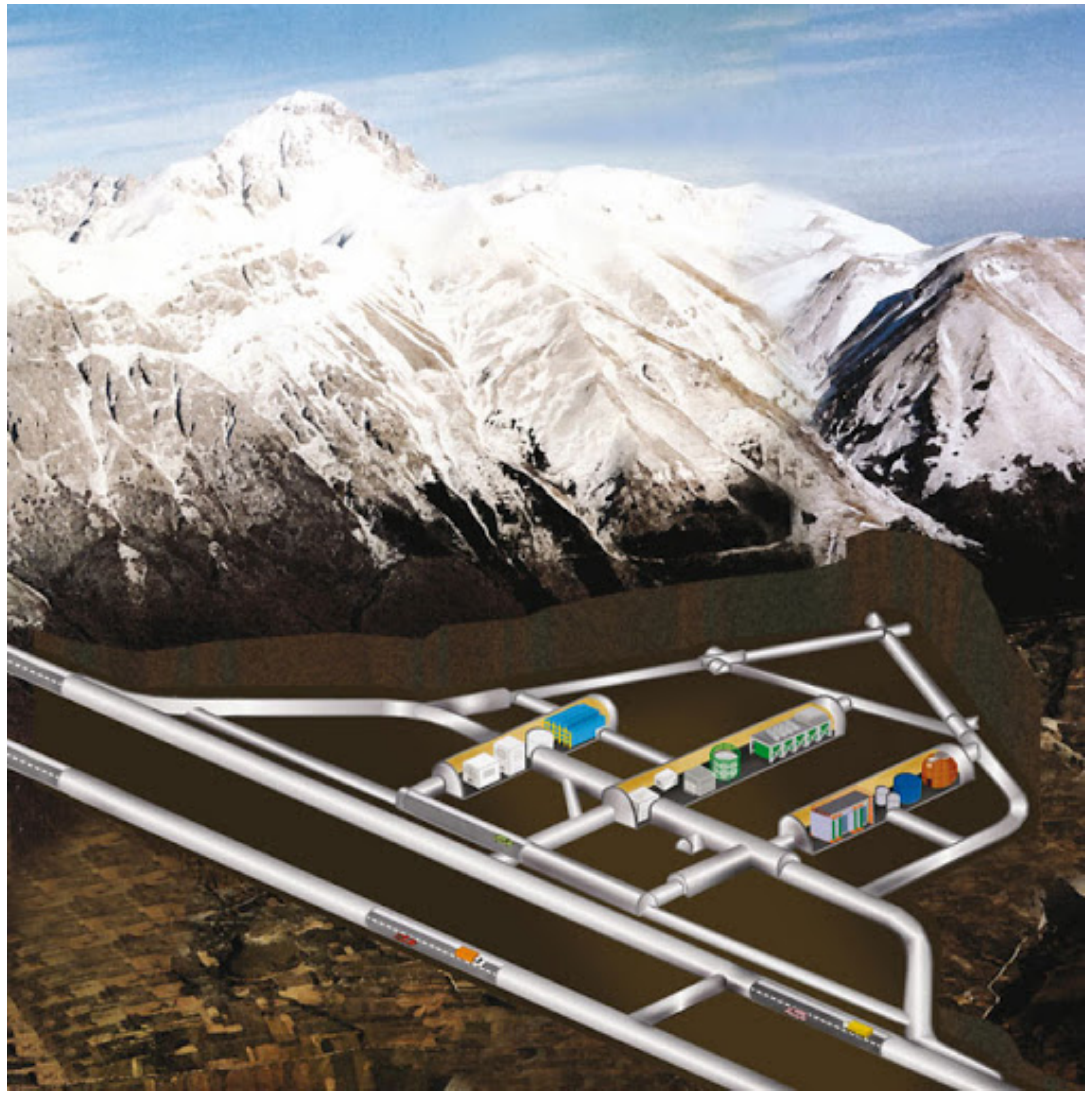
Continuous improvement in relaxation times

Slide material courtesy of Anna Grassellino (FNAL)

SQMS focus areas - focus area 1

Materials for 2D and 3D quantum devices

- We will leverage the world’s largest underground laboratory at the Istituto Nazionale di Fisica Nucleare (INFN) Laboratori Nazionali del Gran Sasso (LNGS), with an overburden of 1.4 km of rock to assess the performance of SRF cavities and transmons with the cosmic ray flux suppressed by 6 orders of magnitude in terms of the impact of non-thermal quasiparticles (“quasiparticle poisoning).

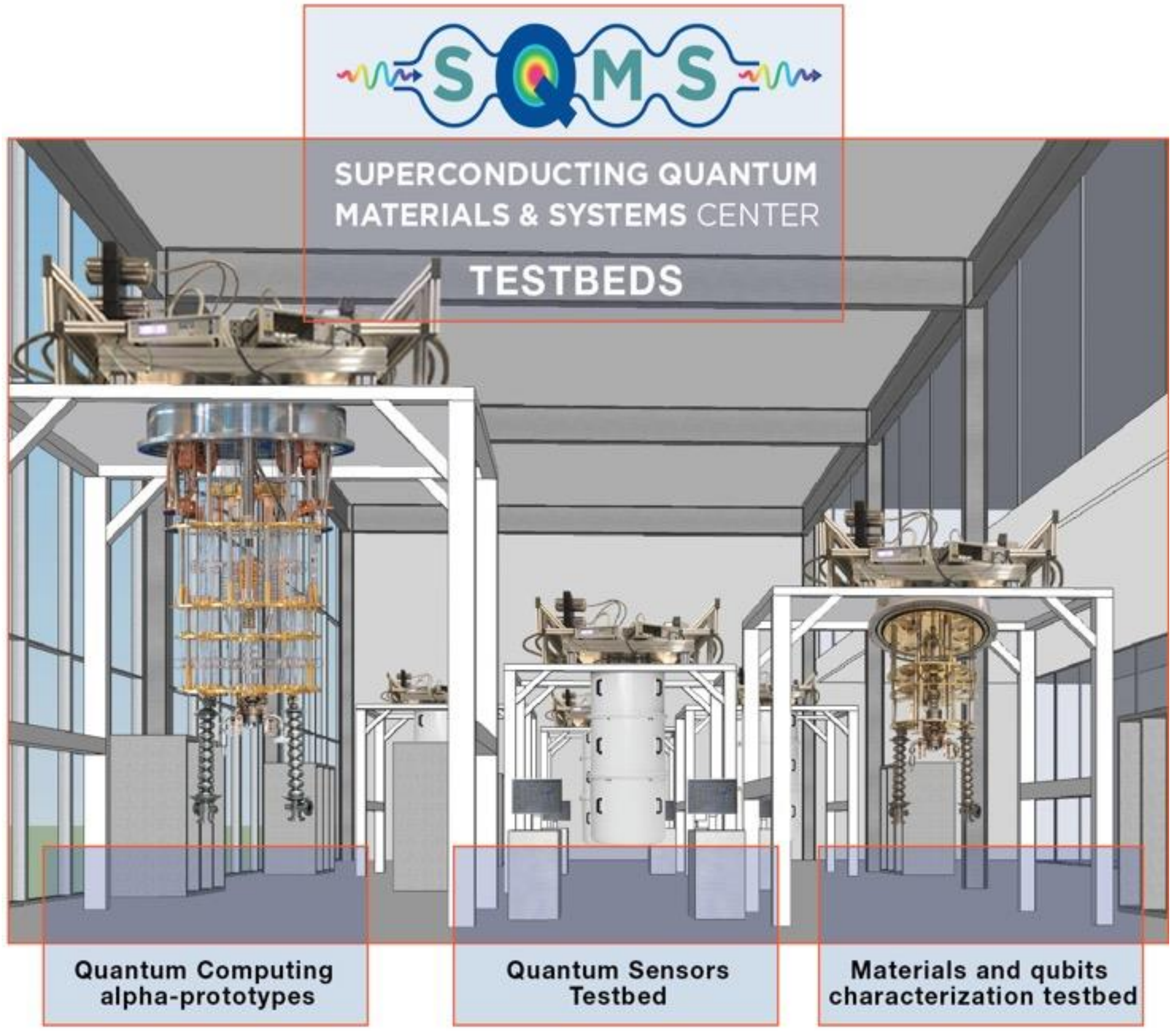


Slide material courtesy of Anna Grassellino (FNAL)

SQMS focus areas - focus area 2

Device integration, prototypes, and QPUs

- Our goal is to build prototype quantum processing units (QPUs) for 2D and 3D superconducting architectures with dramatically increased coherence and size, enabled and propelled by the results of Focus Area 1.
- Within 5 years, we will build a 3D architecture using SRF cavity-based quantum information processors with a target of >200 qubits, all-to-all connectivity, and a coherence time measured in seconds.

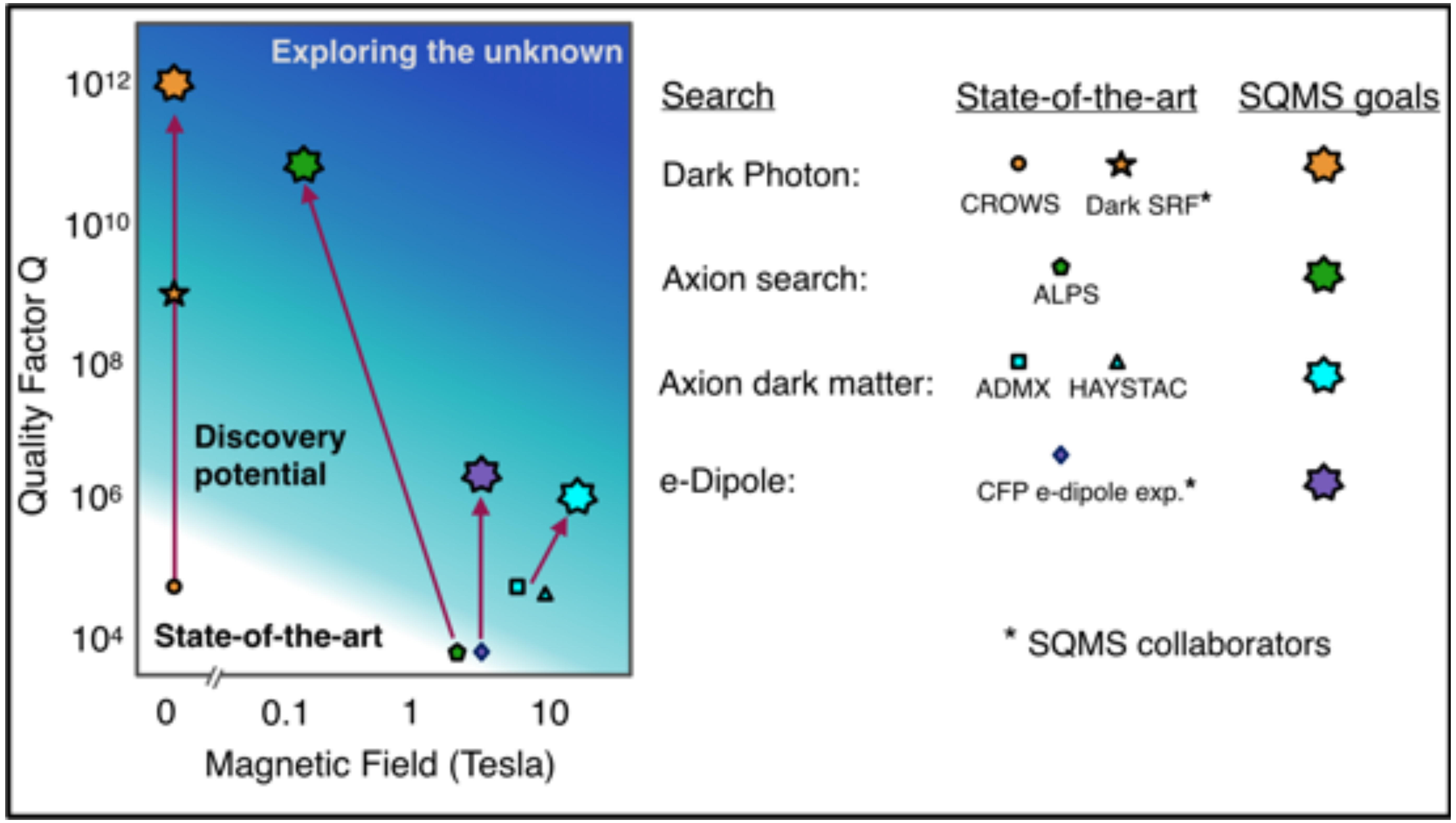


Processor Metrics	Leading Systems	Center Prototypes (3 yr)		Center Device Goals (5 yr)	
		2D-Alpha (estimate)	SRF-Alpha (estimate)	SQMS-2D (estimate)	SQMS-3D (estimate)
Number of qubits	53	128	>100	256	>200
Connectivity graph (qubit:neighbors)	1:4	1:3	1:10	1:3	1:200
Qubit T_1 lifetime, us (median)	70	200	400,000	400	1,000,000
Gate time, ns (median)	20	50	2000	40	100
Coherence/gate time ratio	1,000	4,000	20,000	10,000	100,000,000
Single qubit gate fidelity (%)	99.85	99.6	99.5	99.95	99.95
Two qubit gate fidelity (%)	99.65	99.2	99.5	99.9%	99.95
Achievable circuit depth (1/error)	300	100	200	1,000	2,000

SQMS focus areas - focus area 3

Quantum physics and sensing

- Many interesting opportunities to deploy SQMS technology for fundamental physics experiments.
  - Dark photons
    - Another photon with a different mass - dark matter candidate
    - Common in top-down frameworks
    - Expected to mix with the regular photon
  - Axions and axion-like particles
    - Invoked to solve the strong CP problem
    - Another dark matter candidate - note the synergy between general new particle searches and dark matter searches (lab produced vs natural)



- *And more!* e.g., (g-2)e (penning trap within a cavity), B-L gauge bosons (atom interferometry)

Slide material courtesy of Roni Harnik (FNAL)

SQMS focus areas - focus area 3

Quantum physics and sensing

Why use SRF cavities
for quantum sensing?

Dark SRF: A Dark Photon Search

- High Q cavities allow:
  - Storing a high number of coherent photons.
  - Integrating a coherent signal for long times.

Light Shining through Wall (LSW):

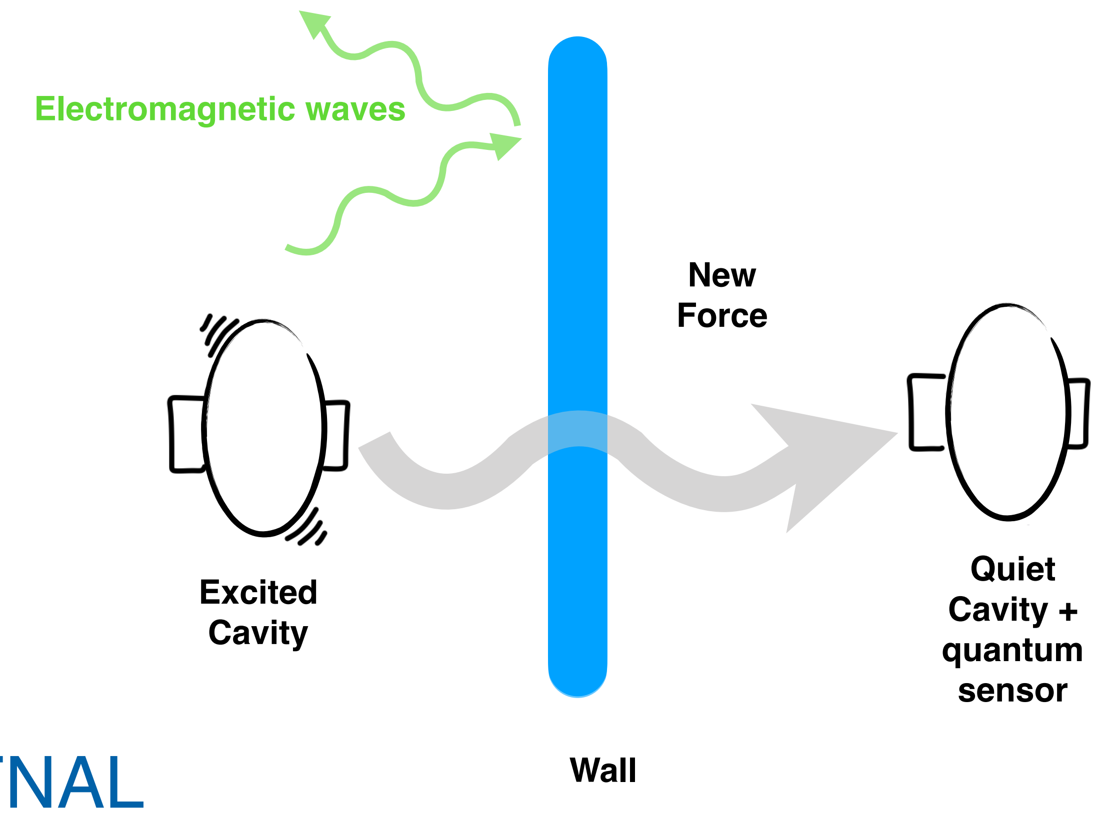
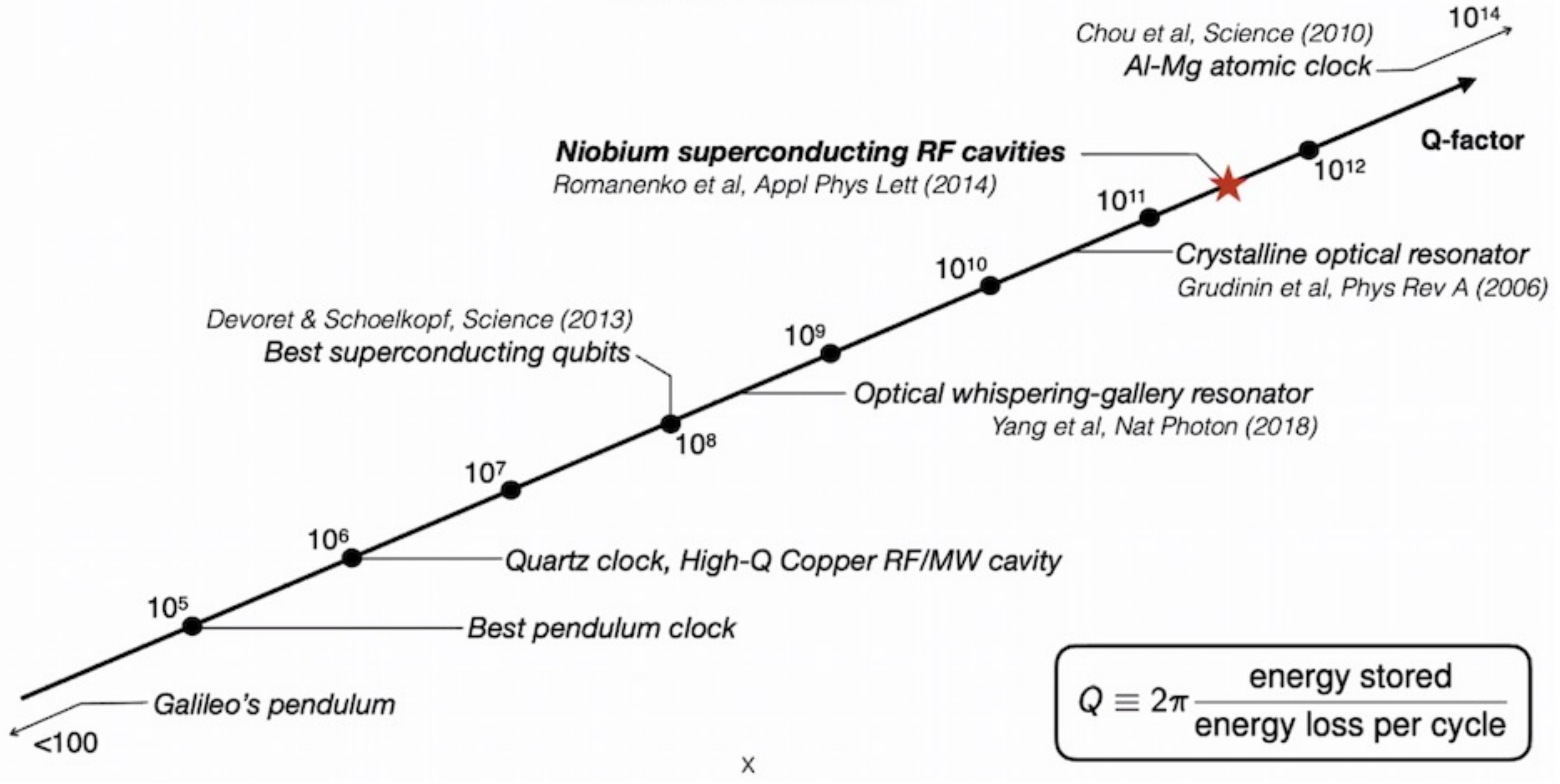


Figure by Roni Harnik, FNAL

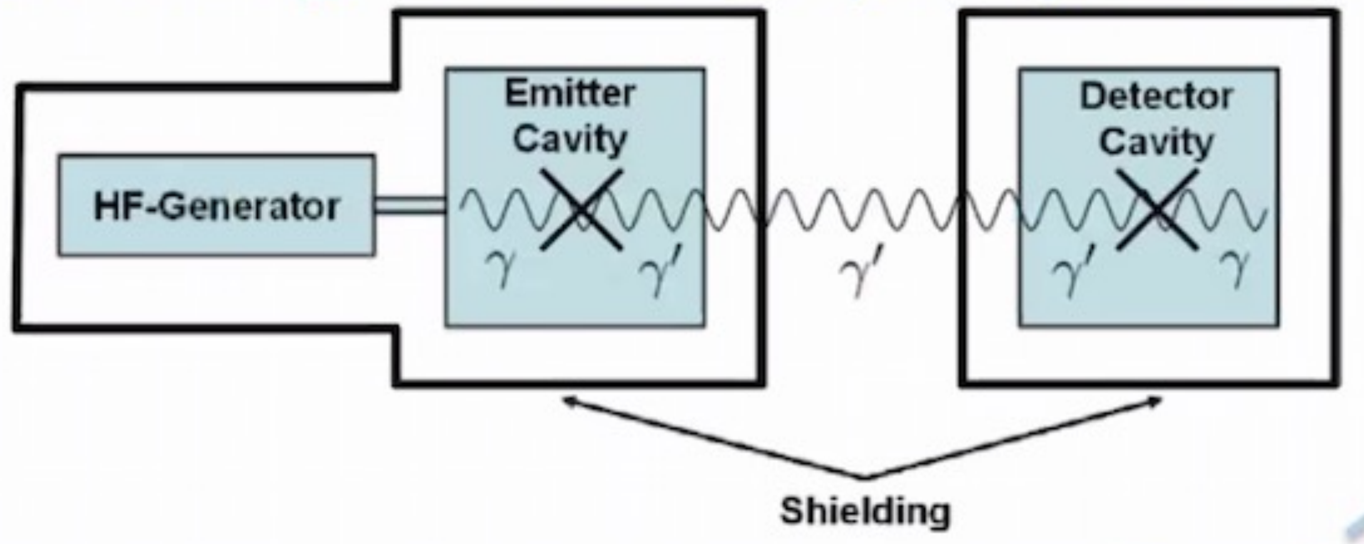
SRF cavities are the most efficient engineered oscillators



S. R. Parker *et al*, Phys. Rev. D 88, 112004 (2013)
J. Hartnett *et al*, Phys. Lett. B 698 (2011) 346
J. Jaeckel and A. Ringwald, Phys. Lett. B 659, 509 (2008)

$Q_{DET}, Q_{EM} < 10^5$ so far used

Looking for hidden paraphotons



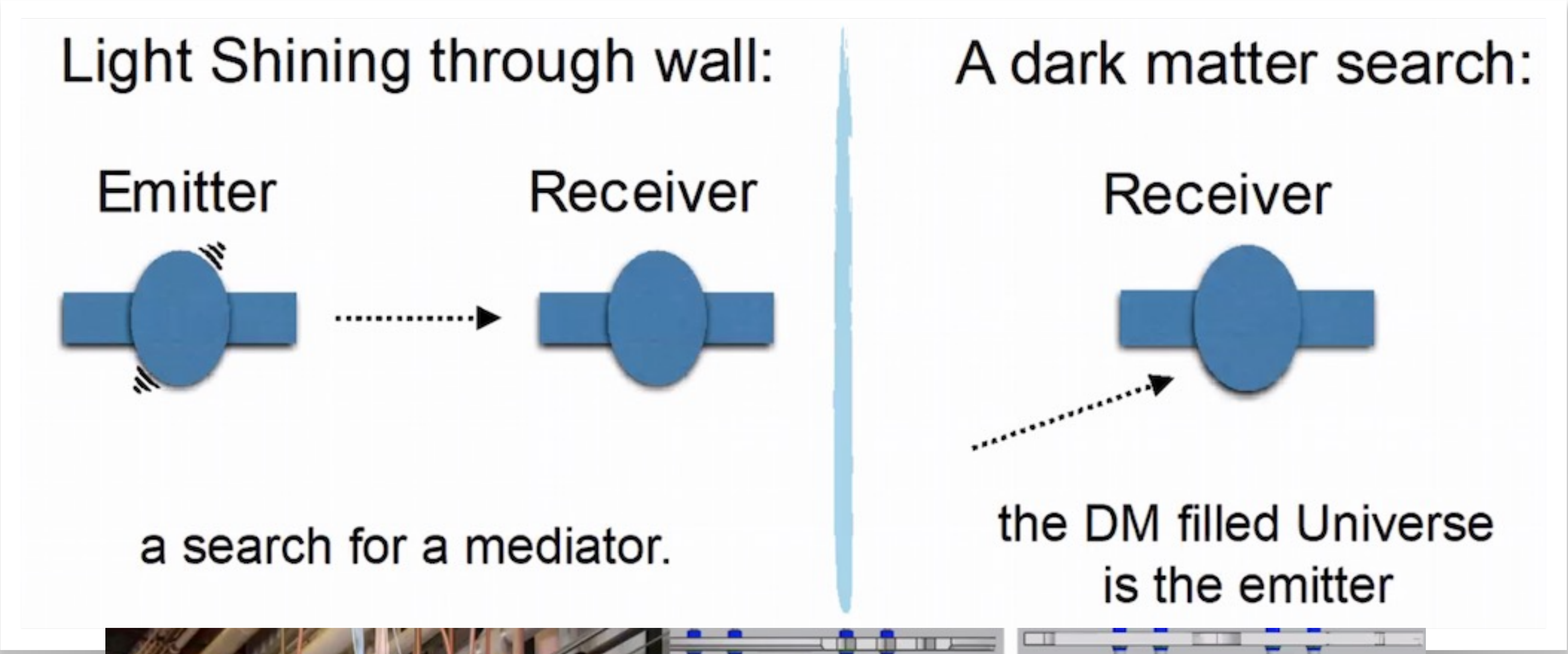
$$\frac{P_{DET}}{P_{EM}} = \chi^4 Q_{DET} Q_{EM} \left(\frac{m_{\gamma\prime} c^2}{\hbar\omega_\gamma}\right)^8 |G|^2$$

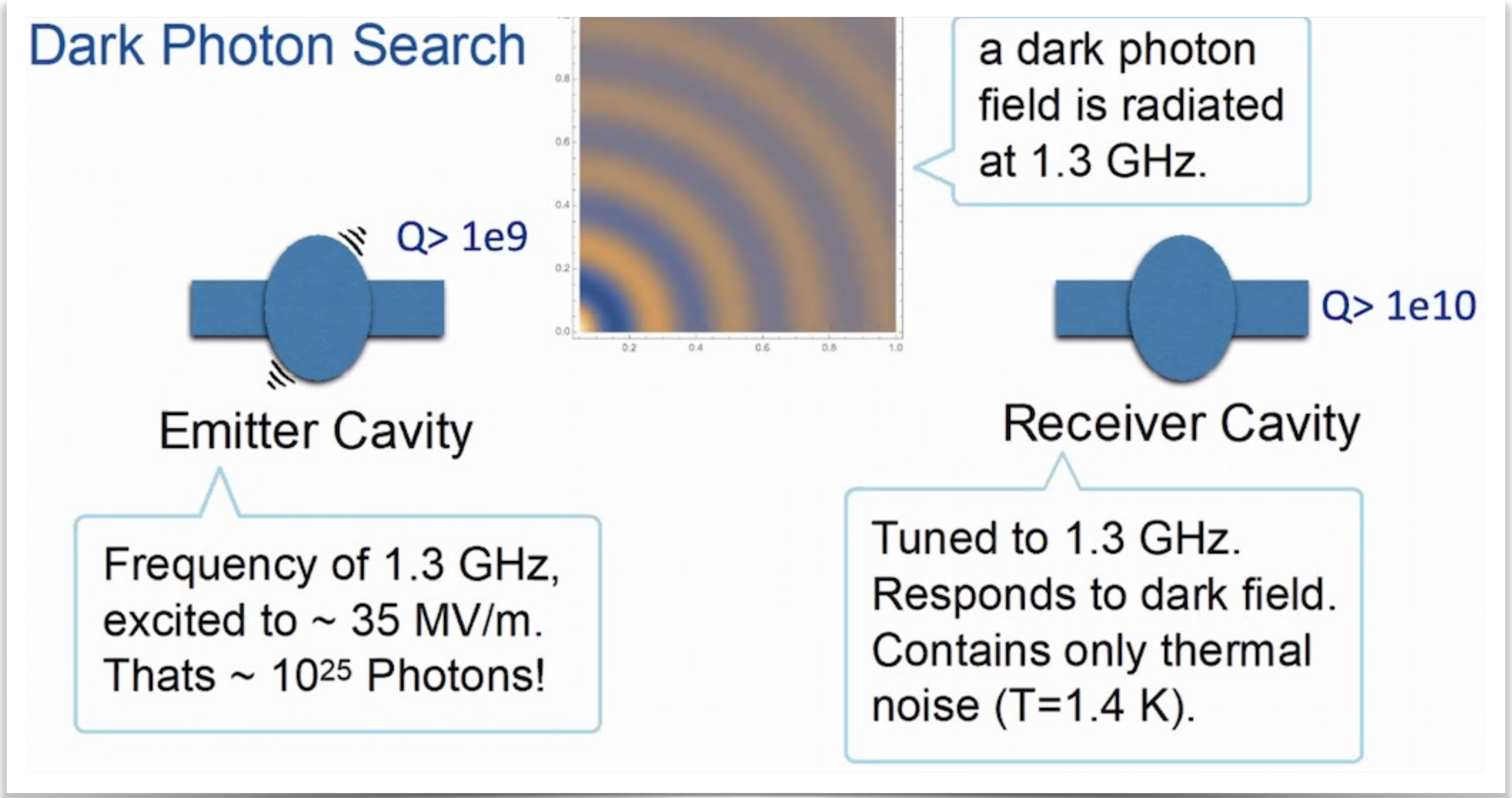
$Q_{DET}, Q_{EM} > 10^{10}$ SRF can offer several orders of magnitude improvement in sensitivity to χ

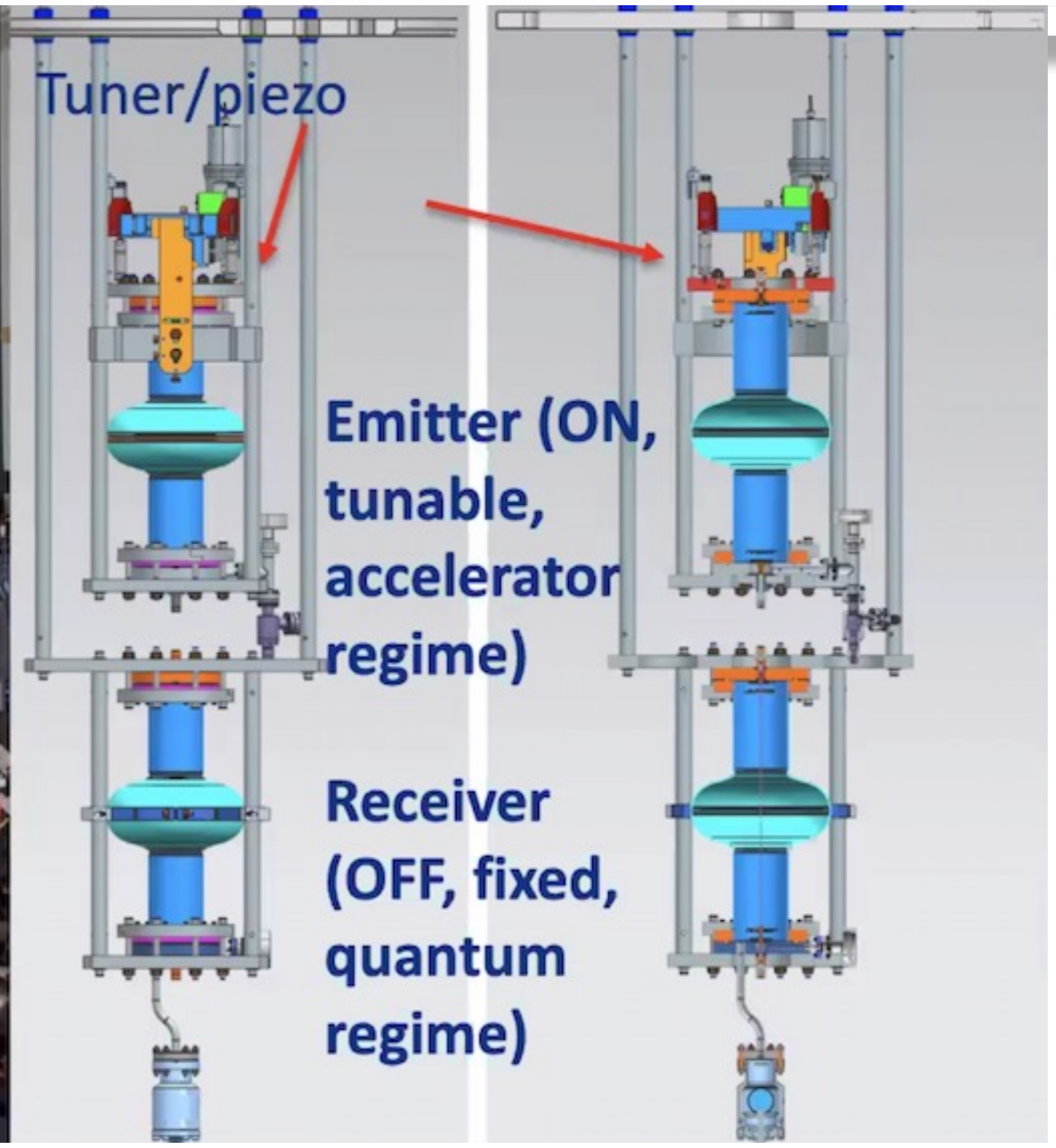
SQMS focus areas - focus area 3

Quantum physics and sensing

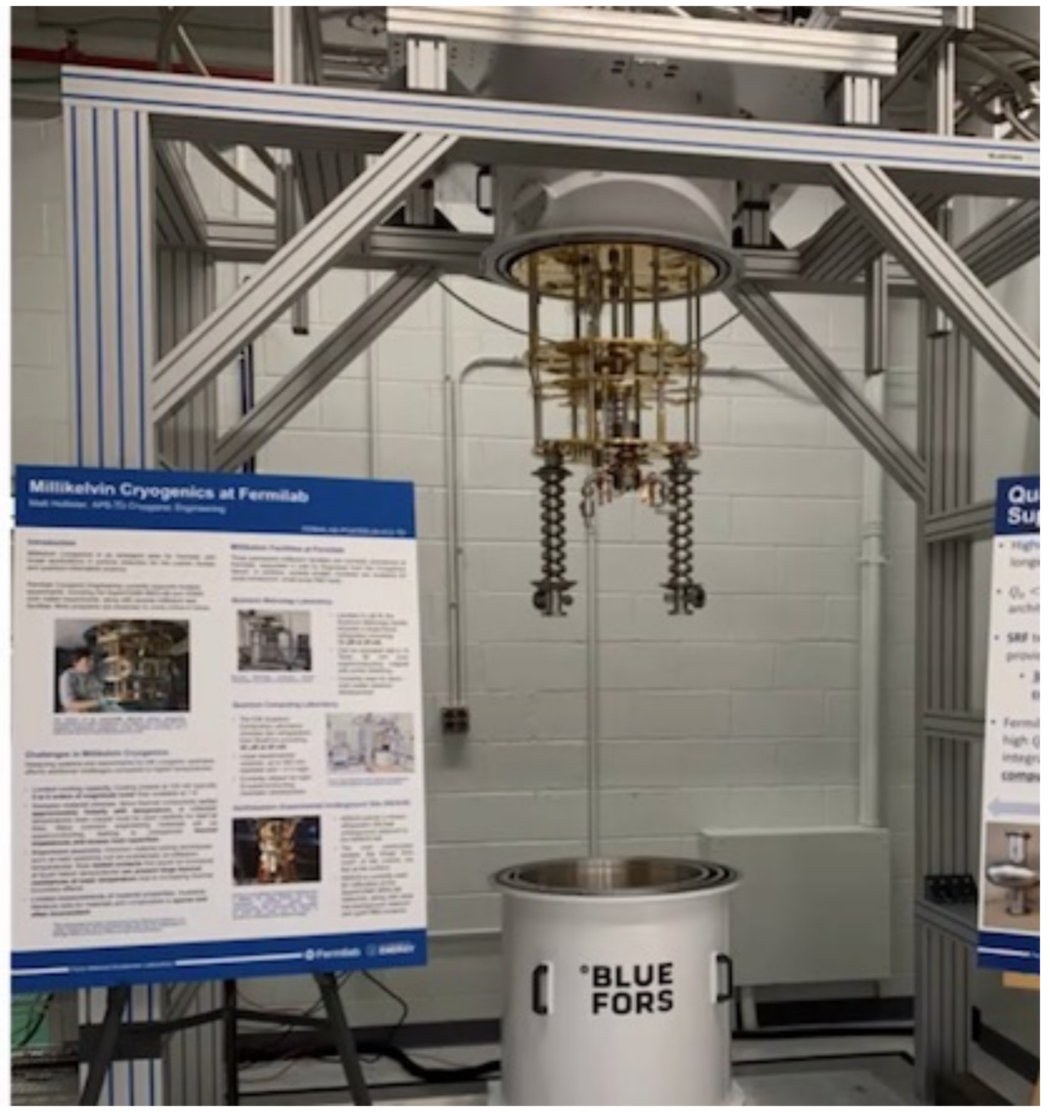
Slide by Alex Romanenko, FNAL







- Designed to sustain several Watts at 2K stage
- Working on transferring the light shine through wall setup to this DR (tuner, piezo, rad shielding…)
- Should be able to run in DR in the next few months

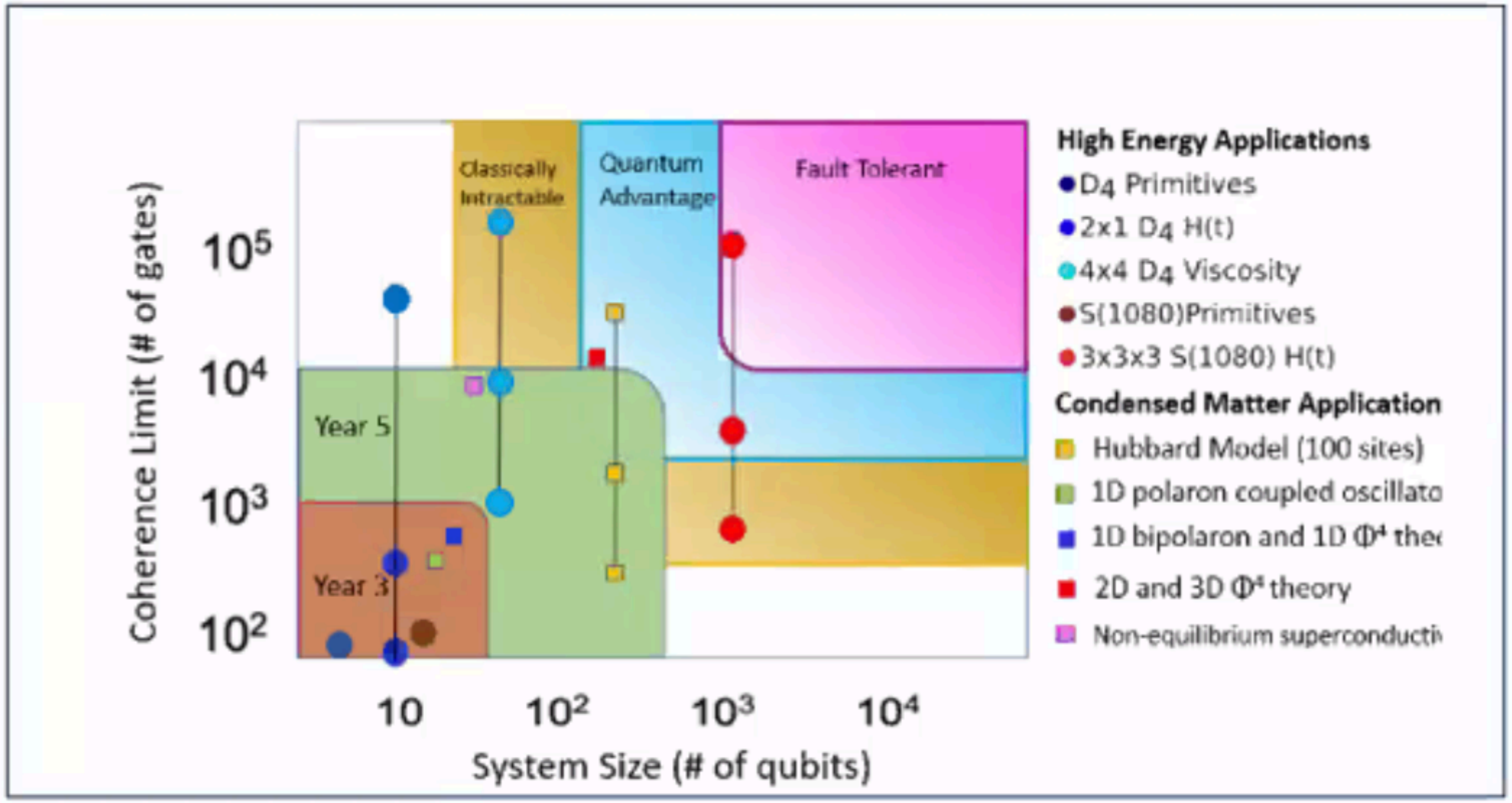


SQMS focus areas - focus area 4

Quantum algorithms, simulation, and benchmarking

- Working across HEP, Condensed Matter Physics, and benchmarking

- Strong synergy in HEP, CMP physics applications (field theory!)
- “2D” platform (array of transmons) and “3D” platform (transmons coupled to cavities) - 2D is ahead for applications.
- 3D work involves more fundamental efforts in gate design and optimization (should we even make gates?), compiler, software stack, etc.
- Open quantum system simulators are a key part of early efforts.



Fermilab

SQMS ecosystem

- The SQMS is built to support national goals in economic competitiveness, security, and sustained leadership in QIS.
- Tech transfer, workforce development, partnerships with small business, etc. are all built into the fabric of the Center.

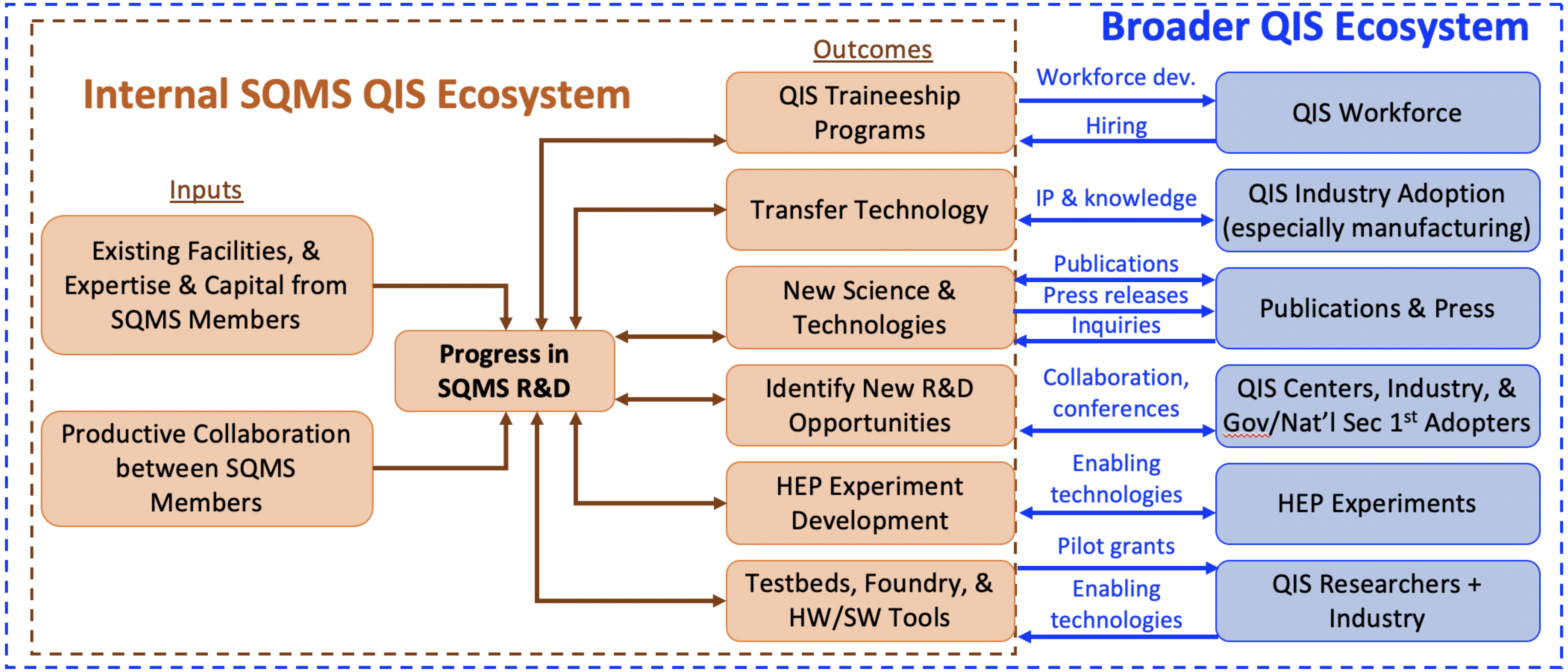


Figure by Mandy Birch, Rigetti Computing

FQI

https://quantum.fnal.gov

FQI

- The Fermilab Quantum Institute is a new(ish) part of the overall lab organization.
- Organized into two thrust areas - Science and Technology (lots of science and technology in both areas)
  - Theory (especially HEP simulation)
  - Superconducting RF
  - Sensing (skipper CCDs, dark photons and axions)
  - Atom interferometry
  - Control electronics
  - Cryogenics
  - Quantum networks
  - Quantum algorithms (HEP applications)
  - Infrastructure (e.g. HEPCloud)

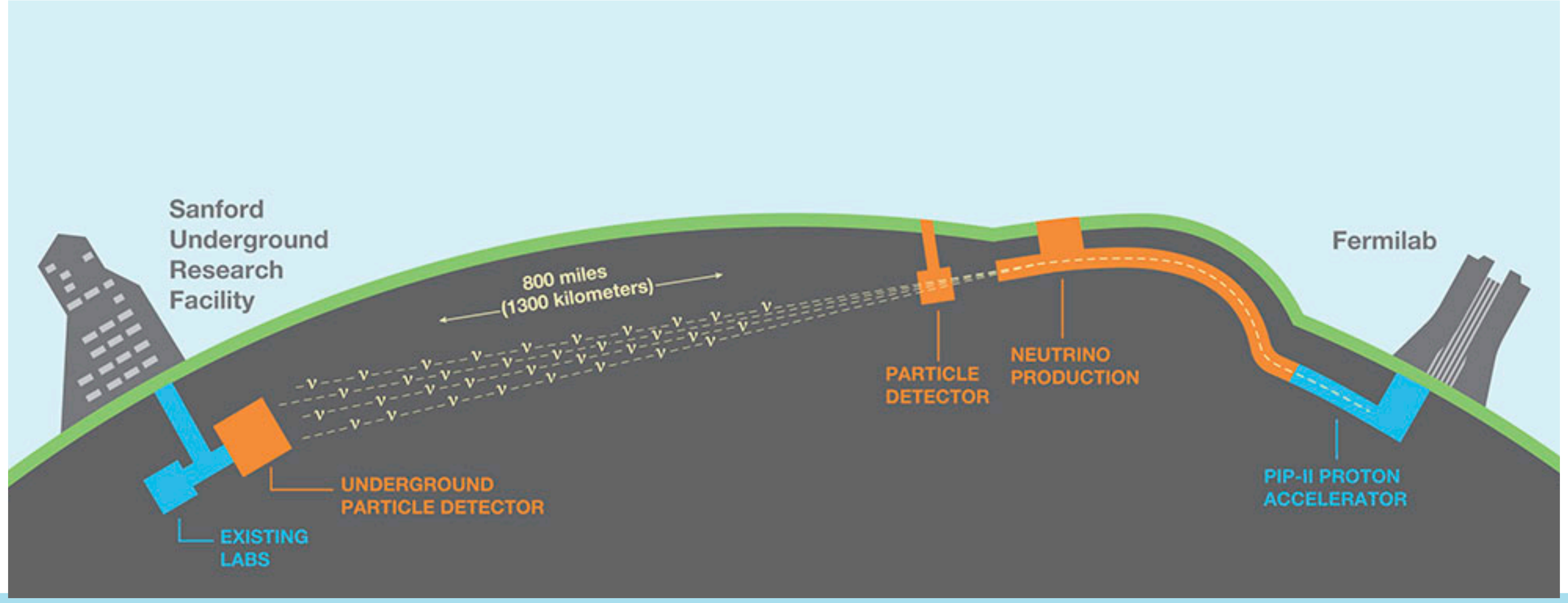
Also w/ industry partners, e.g. Google: https://arxiv.org/abs/2101.09581

Large number of activities, primarily funded by HEP QuantISED program - migrating towards a “base program.”

Activities are synergistic with the SQMS, but *distinct*.

Example application: Neutrino-nucleus scattering

- Cross section systematics are expected to (eventually) be the dominant error at long baseline neutrino oscillation experiment (e.g. DUNE).
- Very challenging theory problem!
  - "On classical computers, inclusive scattering in ab-initio calculations are obtained via imaginary-time (Euclidean) correlation functions or in factorization schemes… **Exact treatments, even for the ground state, scale exponentially in the nucleon number due to the Fermion sign problem.** Constrained path algorithms are useful for low-lying states, but scattering has proven to be intractable on classical computers."
- Can we simulate the process using a quantum computer?



For more, detail, see:

https://link.aps.org/doi/10.1103/PhysRevD.101.074038

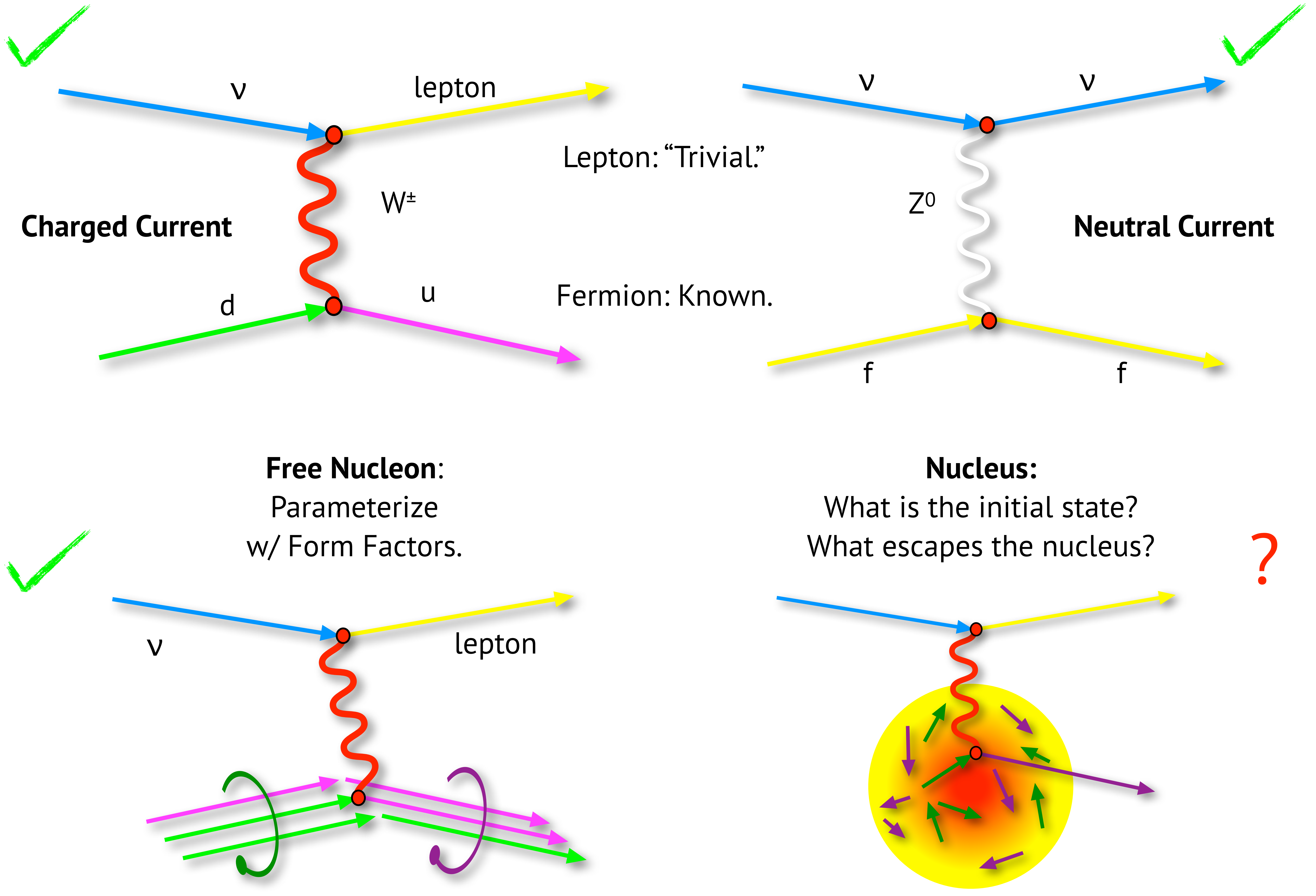
A. Roggero, A. C. Y. Li, J. Carlson, R. Gupta, GP

B. PRD 101, 074038 - 2020

Funded by DOE QuantISED

Why is computing a neutrino cross section so hard?

- There is a hierarchy of challenges.
- Scattering on bare fermions is under control, as is scattering on free nucleons once we measure the nucleon form factors.
- Dealing with nuclear targets is more challenging:
  - We need further theory work to describe the nucleus,
  - The theories we have are too expensive to make computations with, forcing approximate methods.



Why is computing a neutrino cross section so hard?

- What do we mean when we say the nuclear theory is computationally expensive?
  - The quantum many-body problem requires a basis set with an exponentially scaling dimension. Parenthetically, this is also why it is challenging to simulate a quantum computer with a classical computer - we need a Hilbert space of size 2^N, where N is the number of qubits.
  - We would like to use probabilistic methods (Monte Carlo integration) to simulate our quantum system, but we face an important difficulty:

$$i\hbar \frac{\partial |\Psi\rangle}{\partial t} = H|\Psi\rangle \qquad |\Psi(t)\rangle = e^{-i\Delta t H/\hbar} e^{-i\Delta t H/\hbar} \cdots e^{-i\Delta t H/\hbar} |\Psi(0)\rangle$$

  - On the RHS of the second equation, interference problems abound: integrands are not always positive and as *t* grows the integrand fluctuates more and more rapidly. This approach cannot work on classical processors.

Why is computing a neutrino cross section so hard?

- We may make a clever substitution, "Wick's rotation" and find:

$$t \rightarrow -i\hbar\tau \qquad |\Psi(\tau)\rangle = e^{-\Delta\tau H} e^{-\Delta\tau H} \cdots e^{-\Delta\tau H} |\Psi(0)\rangle$$

- This enables fairly accurate MC simulations of time-reversal-invariant systems of interacting bosons - but, we still cannot handle systems of interacting fermions (or bosons with complex hermitian Hamiltonians).
  - Need to find a basis in which all the matrix elements of exp(-**Δτ**H) are positive.
  - In fermion systems the MC process causes state exchanges that produce samples that are positive as often as negative (due to anti-symmetrization requirements). Therefore, the statistical error of measured observables grows exponentially fast with system size.
  - Finally, analytically continuing results back to real time (for truly dynamical information) is an ill-posed problem.

Dynamical linear response on a quantum computer

- Simplest quantum dynamics problem - response of a quantum system to perturbations.
- Goal - use quantum phase estimation to calculate the *response function*:

$$S\left(\omega,\hat{O}\right)=\sum_{\nu}\left|\langle\phi_\nu\left|\hat{O}\right|\phi_0\rangle\right|^2\delta\left(E_\nu-E_0-\omega\right)$$

- QPE is an algorithm to estimate the phase o the eigenvector of a unitary operator:

$$\hat{U}|\phi_\nu\rangle=e^{2\pi i\theta_\nu}|\phi_\nu\rangle$$

$$|\Psi\rangle=\hat{V}_{QPE}|\phi_\nu\rangle|0\rangle_A=|\phi_\nu\rangle|\theta_\nu\rangle_A$$

  - $|\theta_\nu\rangle$: θ_ν stored in ancilla qubits
  - measure ancilla qubits to obtain θ_ν

$$H=-t\sum_{\sigma=1}^{2}\sum_{\langle i,j\rangle}^{M}\left(c_{i,\sigma}^{\dagger}c_{j,\sigma}+c_{i,\sigma}c_{j,\sigma}^{\dagger}\right)+U\sum_{i=1}^{M}\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}\ ,$$

2D fermionic system with Hubbard Hamiltonian; simulated with A=2 nucleons and M=31^2 lattice sites.

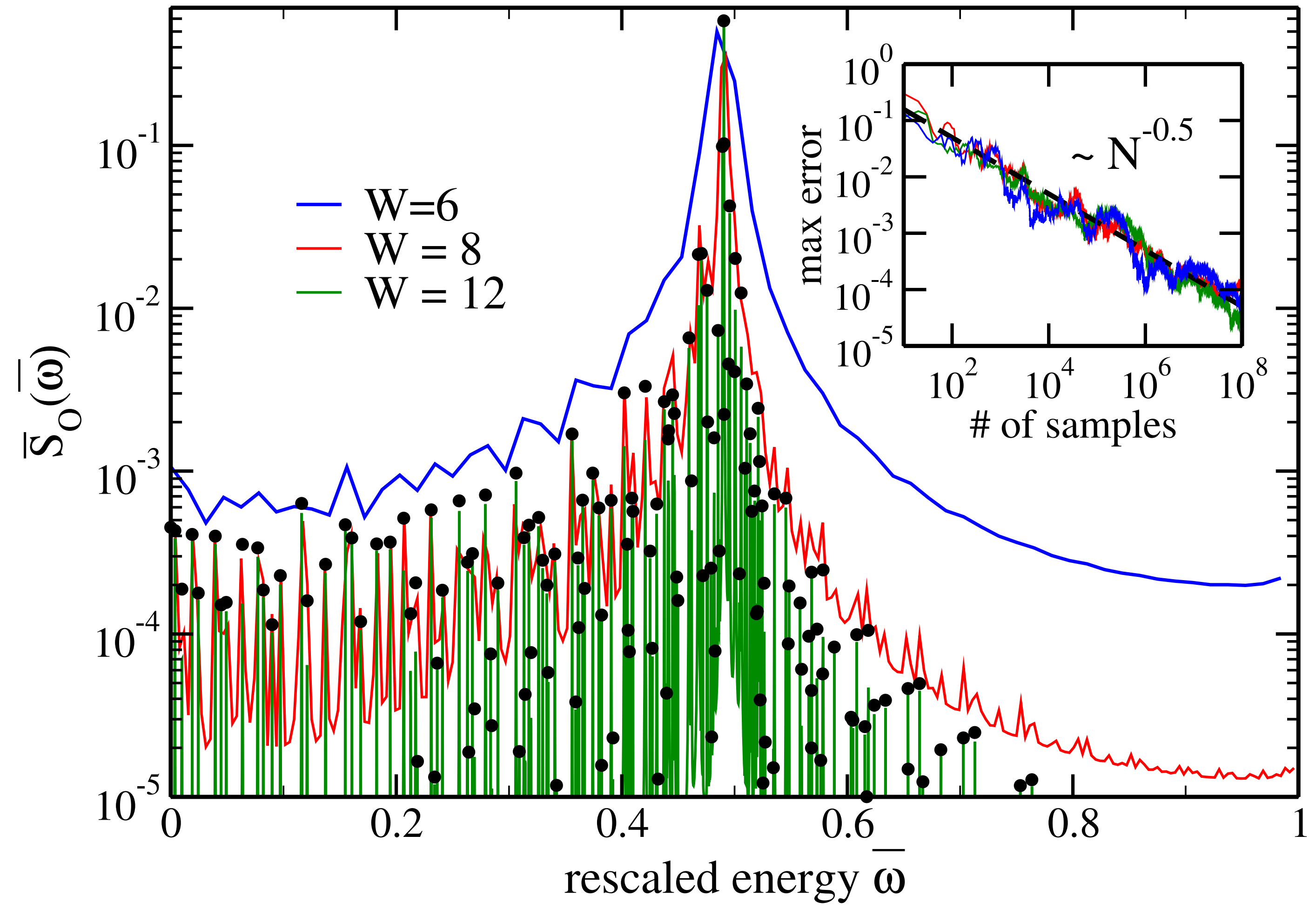
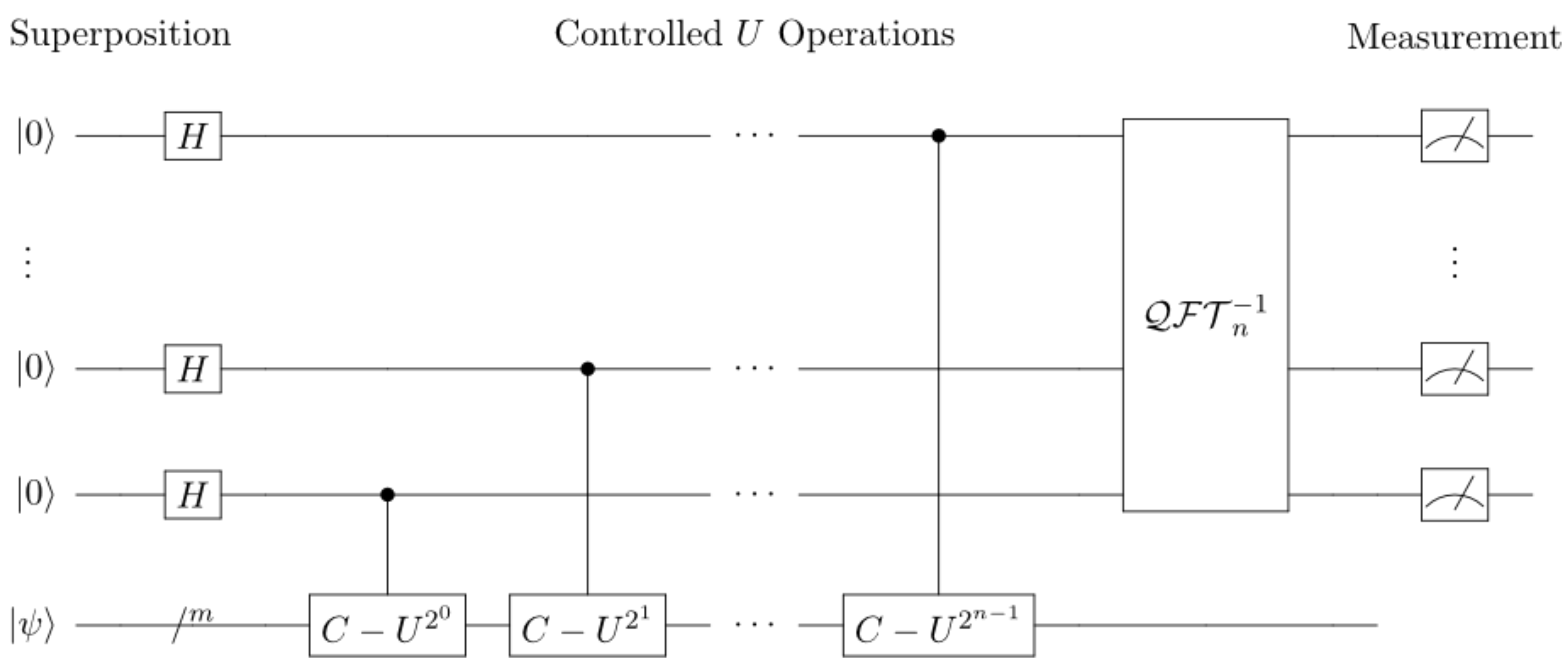


FIG. 1. Approximations of the true response function $\overline{S}_O(\overline{\omega})$ for the model system described by the hamiltonian of Eq. (5) for different numbers of the work qubits: $W=6$ (blue line), $W=8$ (red line) and $W=12$ (green line). The exact response is also shown with black dots. The inset shows the maximum error in the sample estimate of $P(y)$ as a function of the number of samples.

Roggero, A. and Carlson, J. https://link.aps.org/doi/10.1103/PhysRevC.100.034610

Quantum advantage - energy - quantum phase estimation

- The most important subroutine in quantum phase estimation is the quantum Fourier transform.
  - Quantum analog of the inverse discrete Fourier transform.
  - Also used in Shor's Algorithm, computing discrete logarithms, etc. - algorithms for the hidden subgroup problem.
  - Speed-up compared to Fast Fourier transform of N = 2^n numbers:
    - Best classical algorithm: O(n 2^n)
    - Quantum algorithm: O($\log^2$ N) = O(n^2)
      - *Exponential* speed-up! One of the shining applications in quantum computing.



Circuit diagram by Omrika - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=54638138

$$y_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{2\pi ijk/N} x_j$$

Change of basis!

Computational to Fourier bases - controlled rotations (intuition for n^2)

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{2\pi ijk} |j\rangle$$

Quantum advantage - Fermi-Dirac statistics

- Spin systems are very easy to simulate on a quantum computer, but simulating Fermions are hard! Antisymmetrization is challenging.
  - Bosons are actually tough too.
- Antisymmetrization is impossibly expensive on classical resources - algorithms have O(N!) scaling.
- Abrams and Lloyd* proposed an algorithm with *polynomial* scaling - an exponential speedup (and subsequent work does even better).
- The core insight comes from the fact we can create N! states via superposition by rotating each qubit individually (so, O(N) scaling) and then we are able to impose the symmetric group efficiently by leveraging superposition.

* https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.79.2586

See also https://www.nature.com/articles/s41534-018-0071-5 for an improved algorithm.

Aside on bosons

- Two tricky points:
  - Boson number is unbounded

$$\hat{n} = b^\dagger b \rightarrow 0, 1, 2, 3, \ldots$$

  - Physically natural operators, e.g., the lowering operator are difficult to realize with qubits:

$$\begin{aligned} b =& |110\rangle\sqrt{7}\langle 111| \\ &+|101\rangle\sqrt{6}\langle 110| \\ &+|100\rangle\sqrt{5}\langle 101| \\ &+|011\rangle\sqrt{4}\langle 100| \\ &+|010\rangle\sqrt{3}\langle 011| \\ &+|001\rangle\sqrt{2}\langle 010| \\ &+|000\rangle\sqrt{1}\langle 001| \end{aligned}$$

$\Rightarrow$ Useful to have bosons naturally available in your system!

Point from: S. Girvin - https://www.youtube.com/watch?v=miK5y8BYIwQ

Will be exciting to explore these in simulations at the SQMS!

Sketch of the linear response quantum algorithm

$$S(\omega,\hat{O}) = \sum_\nu \left|\langle\phi_\nu|\hat{O}|\phi_0\rangle\right|^2 \delta(E_\nu - E_0 - \omega),\ \hat{H}|\phi_\nu\rangle = E_\nu|\phi_\nu\rangle$$

- Prepare $|\psi_{\hat{O}}\rangle = \frac{\hat{O}|\phi_0\rangle}{\sqrt{\langle\phi_0|\hat{O}^\dagger\hat{O}|\phi_0\rangle}} = \sum_\nu c_\nu|\phi_\nu\rangle$, where $c_\nu = \langle\phi_\nu|\psi_{\hat{O}}\rangle$

Looks kind of like an event generator!

- QPE: $|\Psi\rangle = \hat{V}_{QPE}|\psi_{\hat{O}}\rangle|0\rangle_A = \sum_\nu c_\nu|\phi_\nu\rangle\,|\theta_\nu\rangle_A$, where $\hat{U} = e^{i(\hat{H}-E_0)}$

- Measure ancilla qubits to get probability distribution with readout value ω

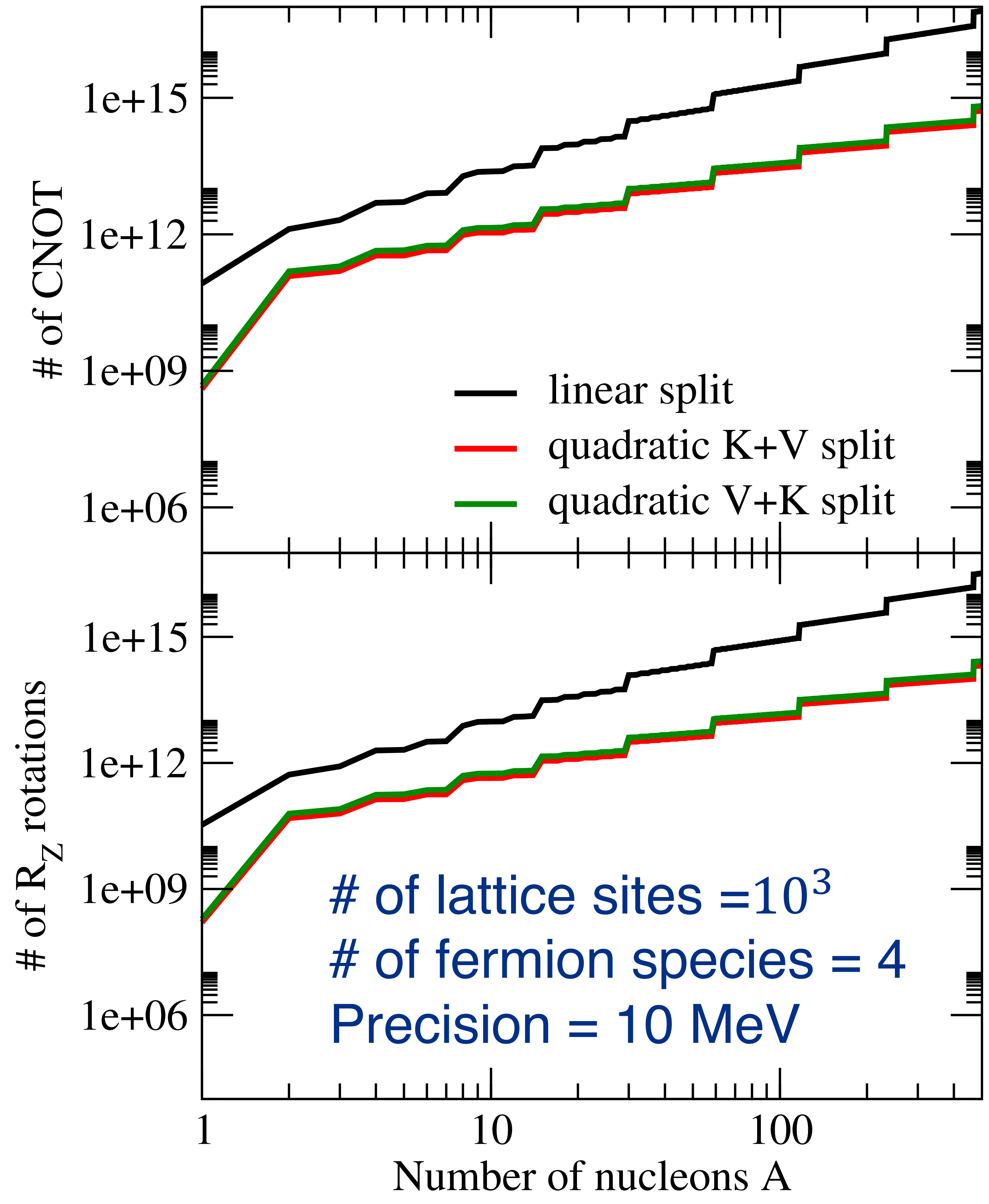
$$P(\omega) = |\langle\omega|\Psi\rangle|^2 = \sum_\nu |c_\nu|^2\,\delta(\theta_\nu - \omega)$$

…GENIE 7.0?

- Put everything back: $P(\omega) = \sum_\nu \frac{\left|\langle\phi_\nu|\hat{O}|\phi_0\rangle\right|^2}{\langle\phi_0|\hat{O}^\dagger\hat{O}|\phi_0\rangle}\delta(E_\nu - E_0 - \omega) = \frac{S(\omega,\hat{O})}{\langle\phi_0|\hat{O}^\dagger\hat{O}|\phi_0\rangle}$

Algorithm sketch and resources

- Full algorithm is impossible on NISQ hardware, but we performed resource estimates, looking at the following:
  - Qubit encoding
    - *A* nucleons on *M* lattice sites with N_f fermion modes per site with Jordan-Wigner: Hilbert space ~ $2^{N_f M}$
    - Lattice location: $A \log_2 M$
  - State preparation
    - Adiabatic state preparation requires many gates, while hybrid variational approaches may face classical optimization challenges
  - Quantum phase estimation
    - Expensive!

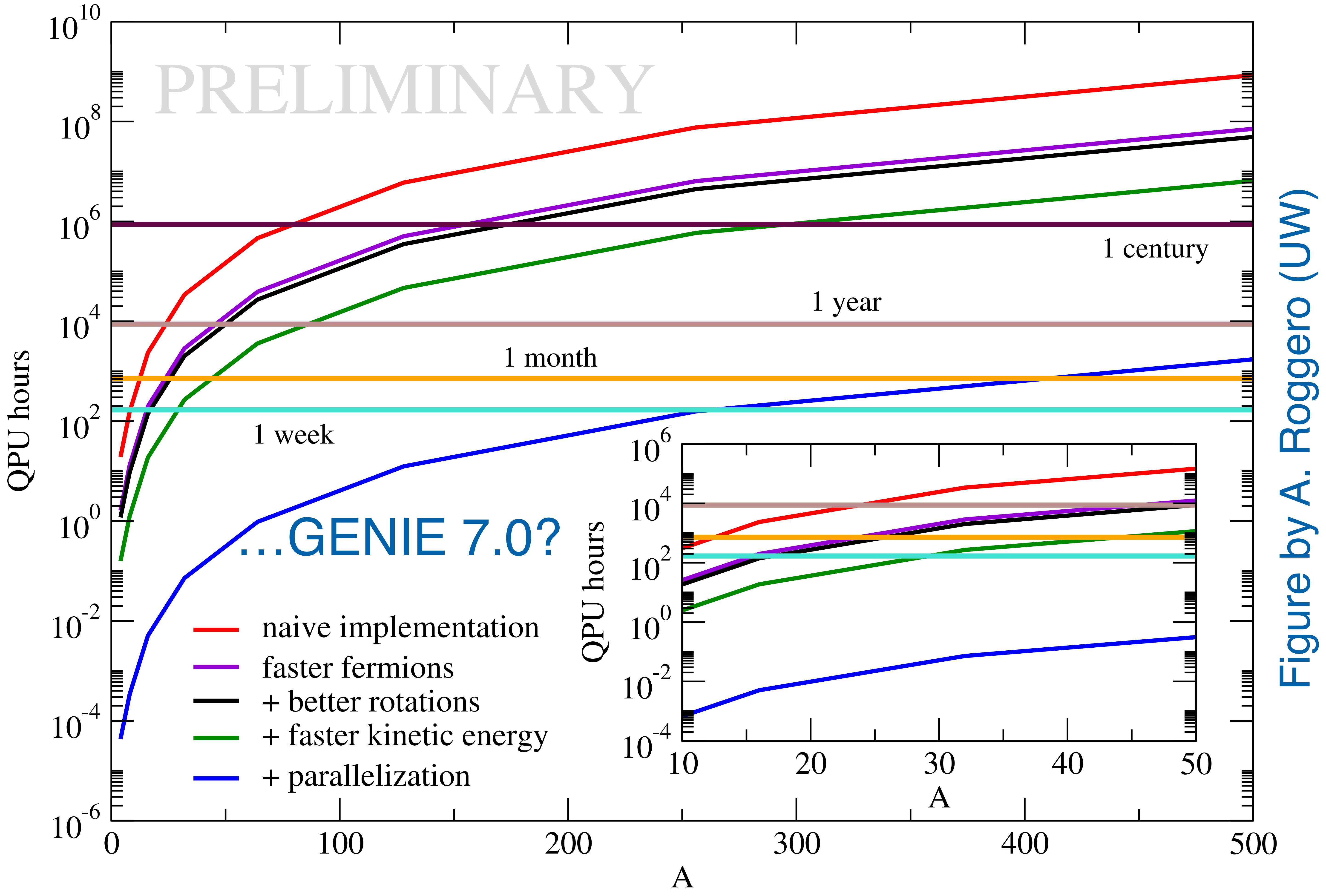


- Gate counts → $\sim 10^{10}$
  - Final 99% fidelity: $e^{\frac{\ln 0.99}{10^{10}}} \rightarrow \sim 10^{-12}$ gate error rate
  - Probably need error-corrected qubits for linear response algorithm with realistic model

Slide material courtesy of Andy Li (FNAL)

A. Roggero et al, https://link.aps.org/doi/10.1103/PhysRevD.101.074038

- Suppose:
  - Use pionless EFT on a lattice with 10^3 points and size 20 fm.
  - Assume 10x faster gates vs. modern state of the art, with no cost for error correction (optimistic).
  - 20 MeV energy resolution
- Require 4000 qubits (current record is ~72, Google roadmap is ~1000 error-corrected qubits in ~10 years).
- Cost for Ar^{40}:
  - Naive ~ O(100) years per momentum transfer value!
  - Optimized ~ 3 weeks per momentum transfer value

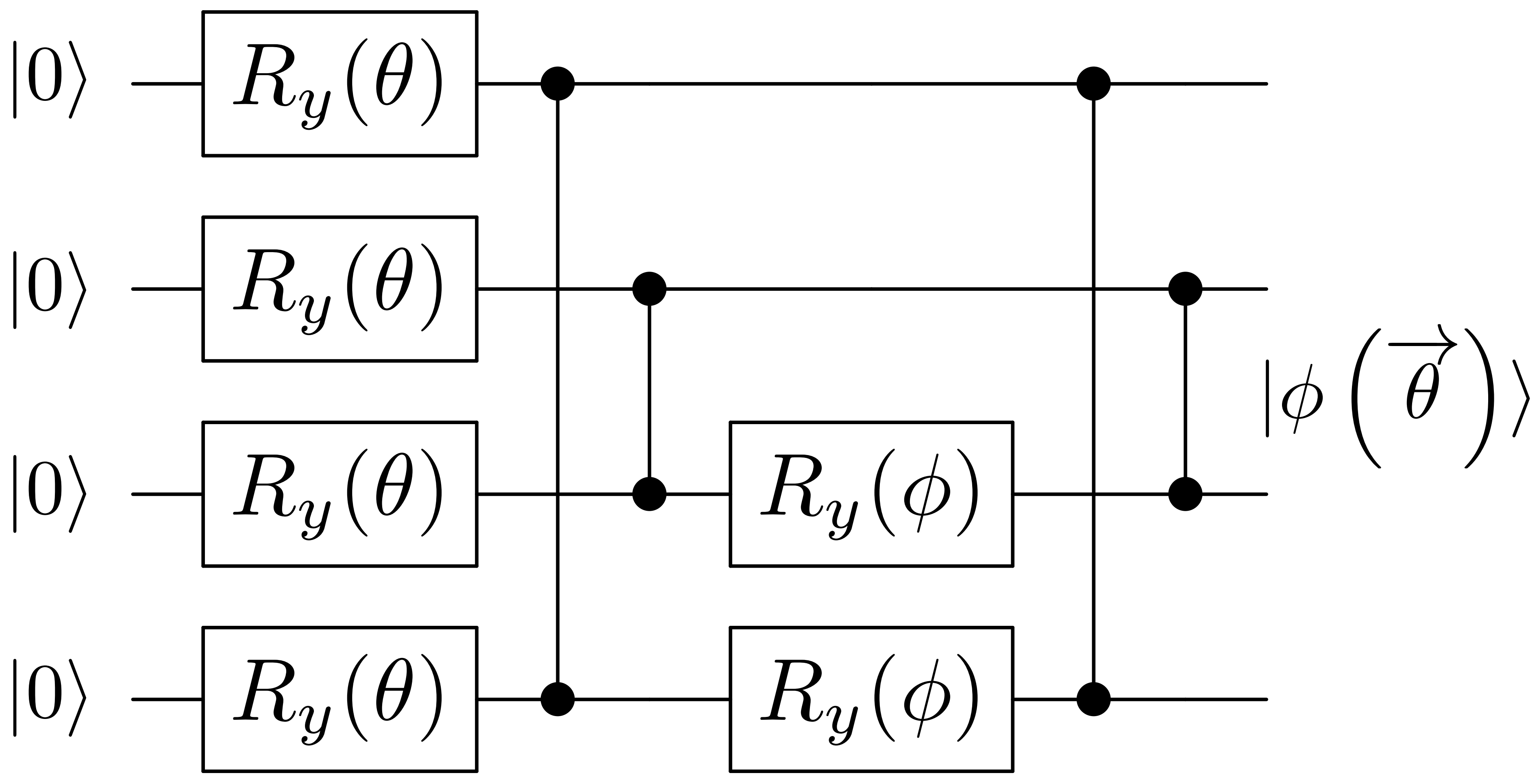


- Algorithm efficiency is critical!
- Best guess is the hardware is ~10-15 years (was "20 years away" for many years 😅)
- Algorithm and theory innovation is critical. We also need to test! (Analog: HPC best algorithms usually lack provable performance guarantees.)

Slide material courtesy of Ale Roggero (U. Washington)

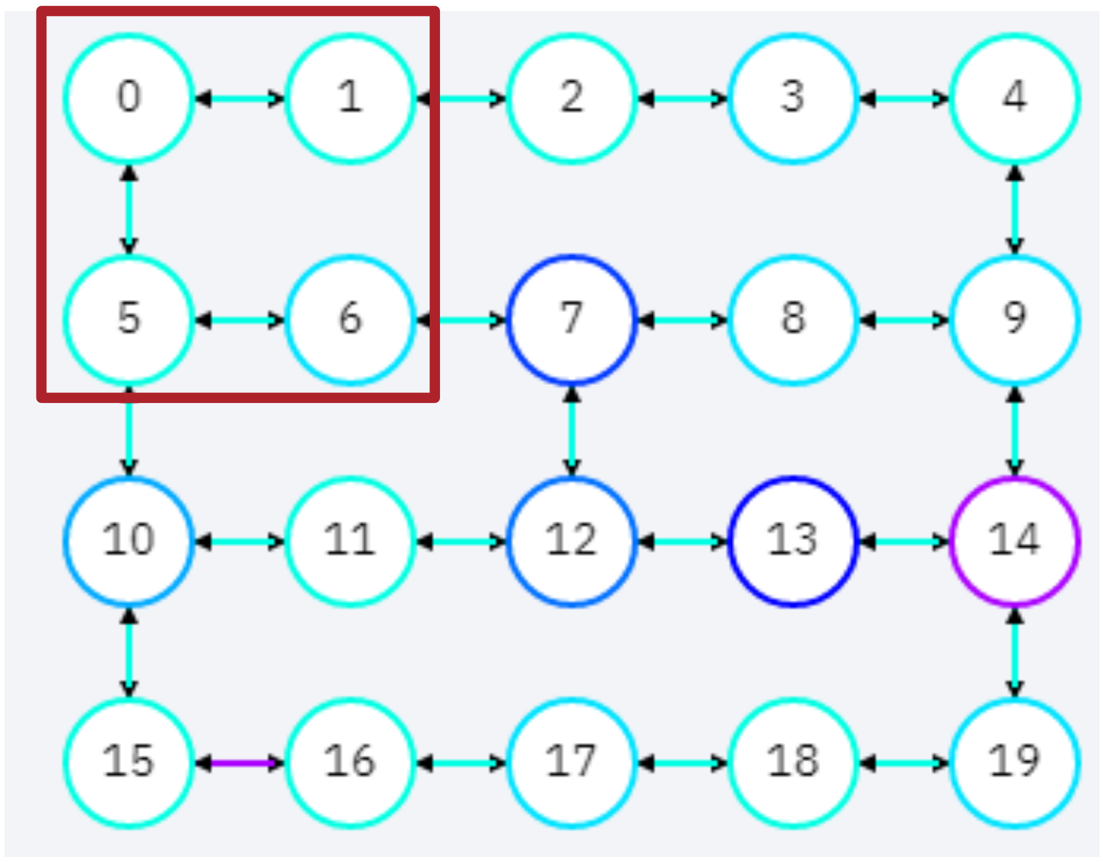
Proof of principle “toy” experiment on four qubits

- Triton toy model: 3 nucleons (with one static, so *A*=2) on a 2x2 (*M*=4) lattice
- Lattice encoding: *A* log *M* = 4 qubits
- IBM Poughkeepsie (1e-3 single qubit error rates, 1e-2 two qubit error rates)
- Ground state prepared by an ansatz optimized with simulation
- Replace full time evolution with a single Trotter step



	Energy	S(0,1)	S(1,0)	S(1,1)
exact g.s.	-4.843	2.038	2.038	2.054
trial state	-4.415	2.024	2.024	2.366
QPU bare	-2.645(15)	2.0290(23)	2.0242(24)	2.1572(25)
QPU corr	-4.4187(98)	1.9993(35)	1.9926(36)	2.2789(51)
QPU sym	-4.322(33)	2.0105(69)	2.0030(45)	2.3341(95)

TABLE II. Results for the ground state energy and the static structure factor. Errors in the experimental result account for statistical fluctuations only.



A. Roggero et al, https://link.aps.org/doi/10.1103/PhysRevD.101.074038

Slide material courtesy of Andy Li (FNAL)

Neutrino-nucleus scattering simulation

- Dynamical linear response function

$$S\left(\omega,\hat{O}\right)=\sum_{\nu}\left|\langle\phi_\nu\left|\hat{O}\right|\phi_0\rangle\right|^2\delta\left(E_\nu-E_0-\omega\right)=\int dt\langle\phi_0\left|\hat{O}^\dagger e^{-i\left(\hat{H}-E_0-\omega\right)t}\hat{O}\right|\phi_0\rangle$$

- $S\left(\omega,\hat{O}\right)\rightarrow$ Inclusive cross sections
- Sample the final state $|\phi_\nu\rangle\rightarrow$ ***semi-exclusive cross sections!***
- Try pointless effective field theory:
  - L. Contessi, A. Lovato, F. Pederiva, A. Roggero, J. Kirscher, U. van Kolck (PLB, https://doi.org/10.1016/j.physletb.2017.07.048) and W. Dawkins, J. Carlson, U. van Kolck, A. Gezerlis (PRL, https://link.aps.org/doi/10.1103/PhysRevLett.124.143402)

$$H=2DtA-t\sum_{f=1}^{N_f}\sum_{\langle i,j\rangle}^{M}\left[c_{i,f}^\dagger c_{j,f}+c_{i,f}^\dagger c_{j,f}\right]$$

Kinetic energy

$$+\frac{1}{2}C_0\sum_{f\neq f'}^{N_f}\sum_{i=1}^{M}n_{i,f}n_{i,f'}$$

Attractive 2-body contact interaction ($C_0<0$)

$$+\frac{D_0}{6}\sum_{f\neq f'\neq f''}^{N_f}\sum_{i=1}^{M}n_{i,f}n_{i,f'}n_{i,f''}\,,$$

Repulsive 3-body interaction ($D_0>0$) to avoid collapse into deeply bound state

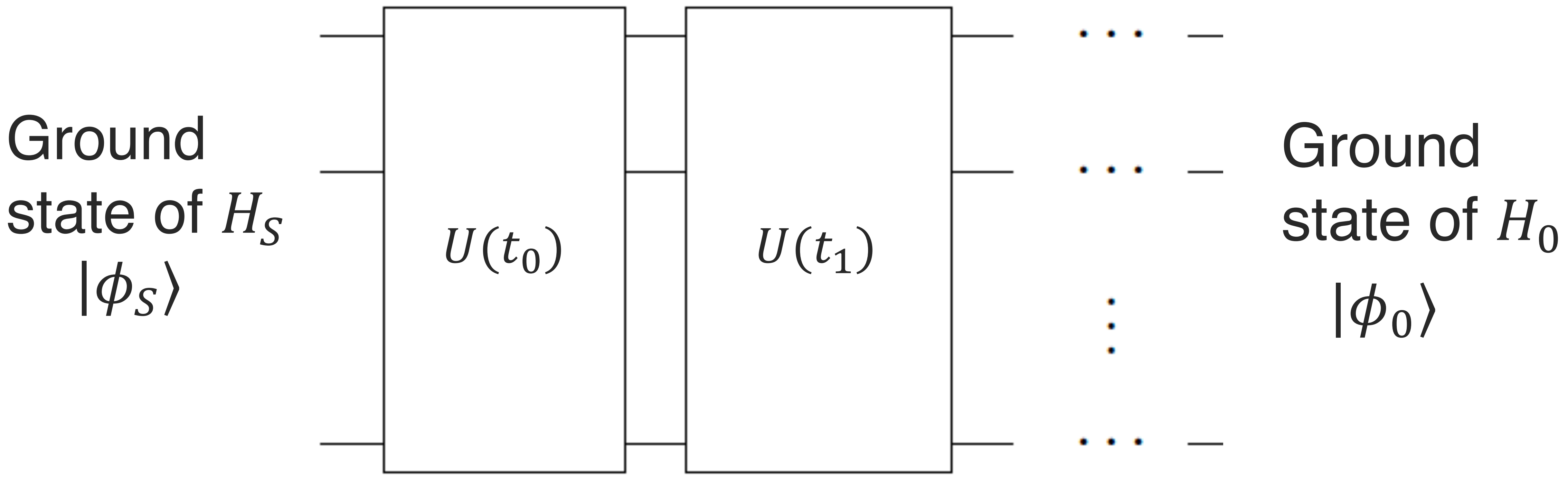
Implementation of ground-state prep. and time evolution

1. Qubit encoding: represent the system by qubits
   - lattice location encoding
2. State preparation: $|\psi_{\hat{O}}\rangle = \frac{\hat{O}|\phi_0\rangle}{\sqrt{\langle\phi_0|\hat{O}^\dagger\hat{O}|\phi_0\rangle}}$
   - Ground-state $|\phi_0\rangle$ prepared by an ansatz optimized by a simulator
3. Quantum phase estimation of $|\psi_{\hat{O}}\rangle$ with $\hat{U} = e^{i(\hat{H}-E_0)}$
   - Time evolution by $\hat{U}(t) = e^{i(\hat{H}-E_0)t}$ on a pretrained initial state
   - Note: $S(\omega, \hat{O}) = \langle\phi_0|\hat{O}^\dagger e^{-i\,(\hat{H}-E_0-\omega)t}\hat{O}|\phi_0\rangle$
4. Measure ancilla qubits: probability distribution $\rightarrow S(\omega, \hat{O})$
   - Direct measurement of qubits representing the particles (no ancilla qubits)

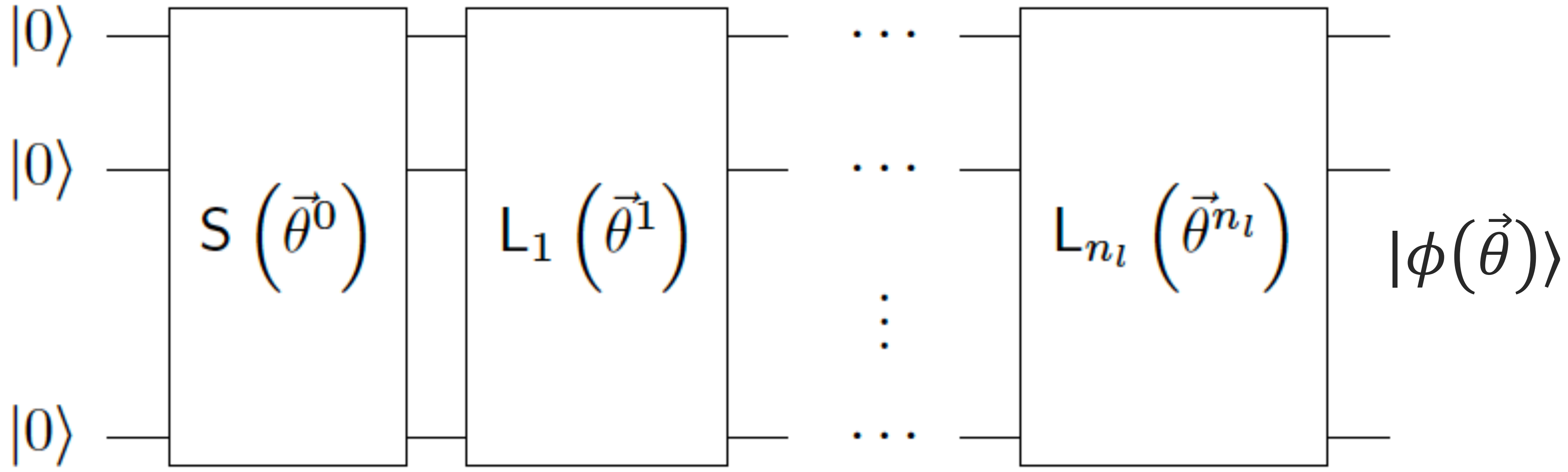
Fermilab

Ground state $|\phi_0\rangle$ preparation algorithms

- Adiabatic quantum state preparation
  - Ground state $|\phi_S\rangle$ of H_S which can be prepared in simple way
  - Evolve $|\phi_S\rangle$ with $H(t) = H_S\left(1-\frac{t}{T}\right) + H_0\frac{t}{T}$ for a duration of time T
  - Many qubit gates (operations) required

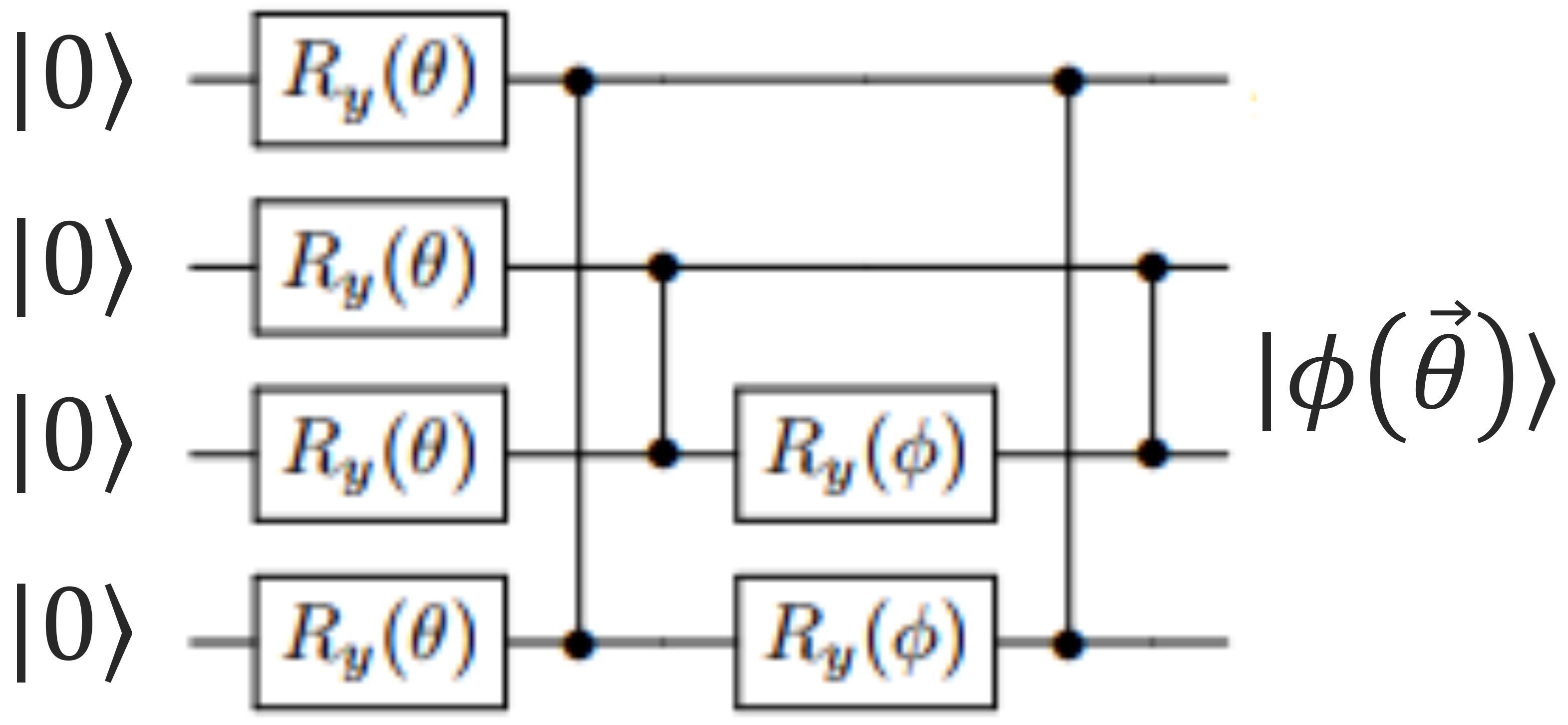


- Hybrid variational state preparation
  - Use a circuit variational ansatz $V(\theta)$ to produce a trial state $|\phi(\theta)\rangle = V(\theta)|0\rangle$
  - Minimize $\langle\phi(\theta)|\widehat{H}_0|\phi(\theta)\rangle$ by a classical optimization algorithm to obtain $|\phi_0\rangle$
  - Small # of qubit gates but classical optimization loop could be expensive



Ground-state prepared by a variational ansatz

- 2-parameter variational ansatz $|\phi(\vec{\theta})\rangle$
- Trained by a noiseless simulator to minimized the energy $E(\vec{\theta}) = \langle\phi(\vec{\theta})|H|\phi(\vec{\theta})\rangle$
- Run the pretrained circuit on the IBM QPU
- QPU shows a promising result with error mitigation (readout noise and CNOT gate fidelity)



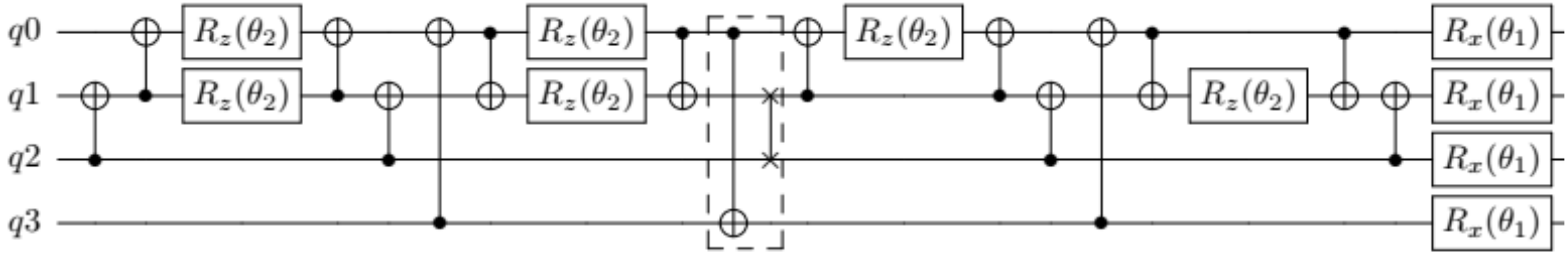
$$H = 8t + \frac{U}{2} - 2t\sum_{k=1}^{4} X_k - \frac{U}{4}(Z_1Z_4 + Z_2Z_3) - \frac{U}{4}\sum_{i<j<k} Z_iZ_jZ_k$$

	Energy
exact g.s.	-4.843
trial state	-4.415
QPU corr	-4.4187(98)

Time evolution with 1 Trotter step

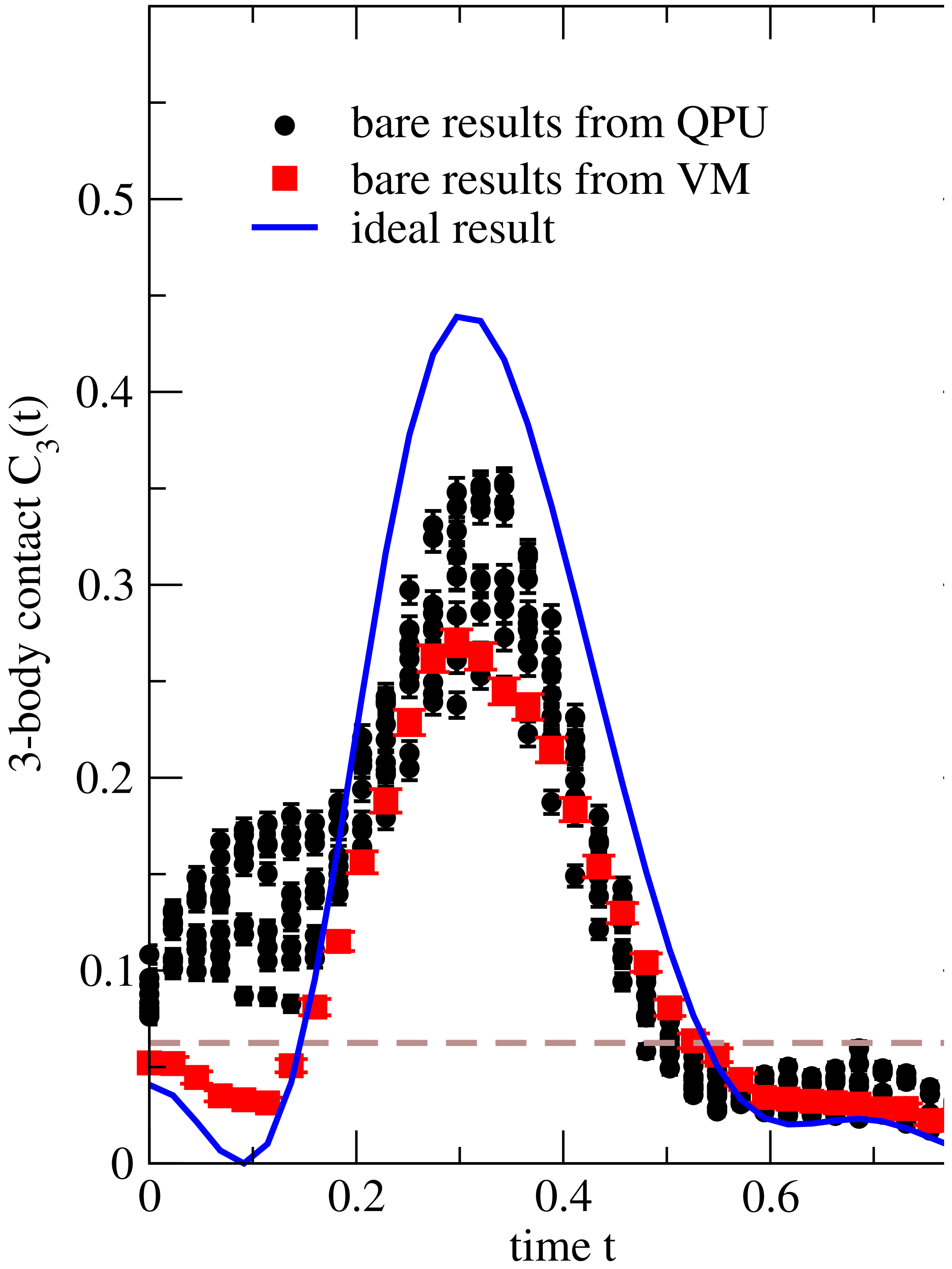
$$H = 8t + \frac{U}{2} \underbrace{- 2t\sum_{k=1}^{4} X_k}_{K} \underbrace{- \frac{U}{4}(Z_1Z_4 + Z_2Z_3) - \frac{U}{4}\sum_{i<j<k} Z_iZ_jZ_k}_{V}$$

- 1st order Trotter's step: $U(\tau) = e^{-i\tau K}e^{-i\tau V}$
- Initial state: pretrained state $|\phi(\vec{\theta})\rangle$
- Time evolve with just 1 Trotter's step $U(t)$
  result deviates from exact significantly when $t > 0.1$ due to Trotter decomposition error
- 3-body contact with : $C_3(t) = |\langle 0000|U(t)\phi_0\rangle|^2$
  $|0000\rangle$: all nucleons at site 1

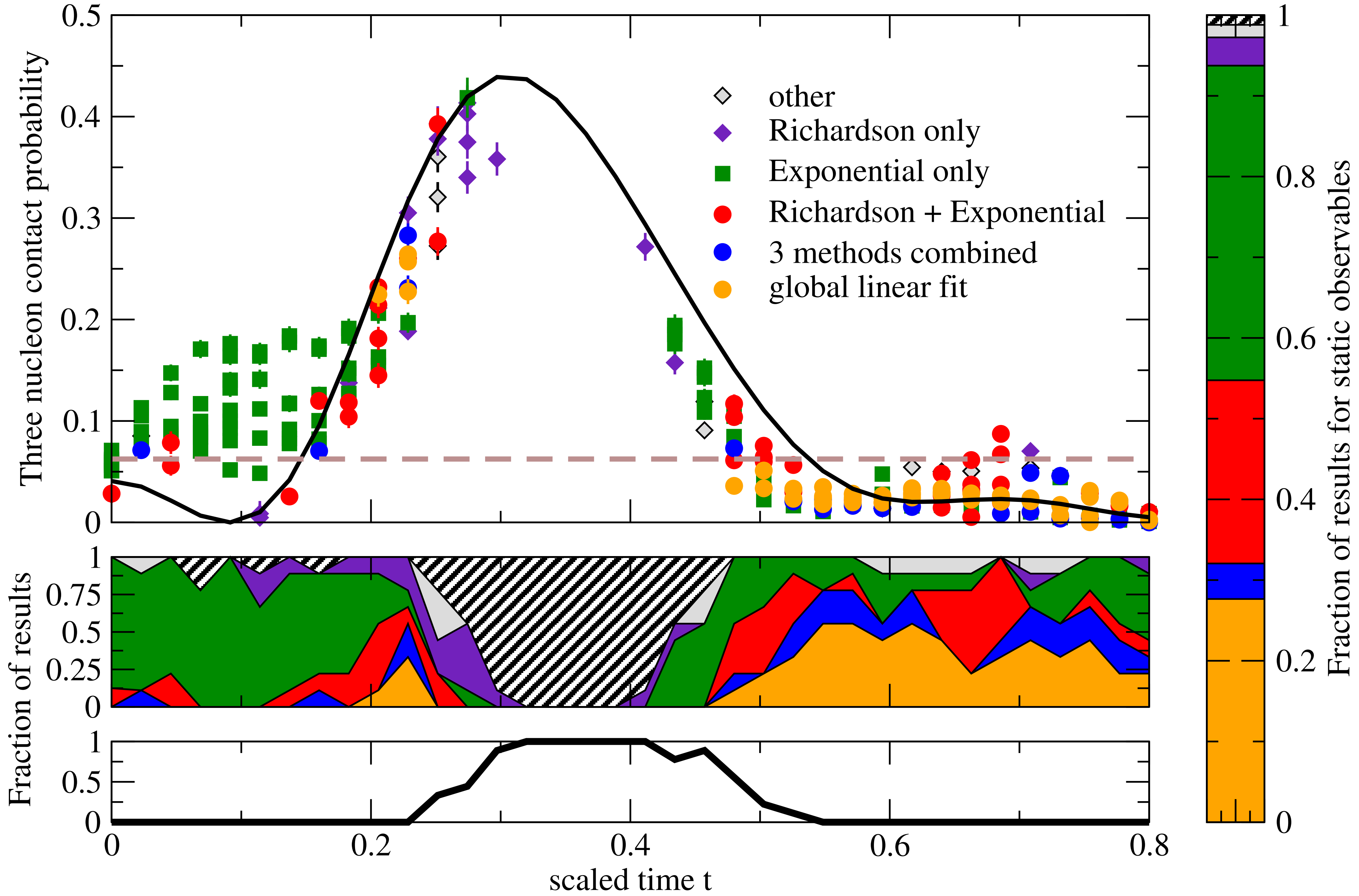


Proof of principle experiment on four qubits - errors

- In small t regime where Trotter decomposition may be used, error from gate infidelity is large, making multiple Trotter steps impossible.
- Error mitigation is not enough to control the issues.
  - Positive: Behavior with circuit depth is what we expect.
- Linear response of simple models may be a near-term application of merit, but we require improvements in error mitigation and hardware.



$$C_3(t) = \langle \Psi(t) | \Pi_{0000} | \Psi(t) \rangle \equiv |\langle 0000 | \Psi(t) \rangle|^2$$



A. Roggero et al, https://link.aps.org/doi/10.1103/PhysRevD.101.074038

Slide material courtesy of Andy Li (FNAL)

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Conclusions

- Quantum computing and quantum technologies have the potential to be powerful tools in the HEP science program.
- Furthermore, HEP has an important and useful role to play in the national quantum science program - in terms of core technologies, applications, and other organizational strengths.
- The SQMS hosted at Fermilab has the ambitious goal of attacking the problem of decoherence at a fundamental level, and combining advances in materials, devices, and algorithms to build a powerful new computing and sensing platform.
- The FQI has a broad and diverse portfolio of activities that show the full spectrum of possibility when HEP and QIS engage productively.
- ***We are always looking for new partners and collaborators!***

Thanks for listening!

SQMS ecosystem

- Early focus areas:
  - Graduate certificate (NU) designed to meet industry asks
  - Summer internships (possibly multi-year)
  - Graduate fellowships (NU, Y2-Y5)
    - Enhanced support & recruit outstanding women and URM candidates
  - Postdoctoral fellowships (Y2-Y5)
    - Named fellowship - Enhanced stipend
    - Research + Diversity + Independence across the Center
  - Summer schools
    - Galileo Galilei Institute in Florence
  - Junior member travel grants
  - Women in Quantum (Y3)
    - 2 day conference modeled on APS CuWiP

Slide material from M. Birch (Rigetti), M. Driscoll (Northwestern), D. Venturelli (NASA)

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SQMS ecosystem

- Summer schools at GGI

Watch for news soon!

The Galileo Galilei Institute (GGI) in Florence is a research hub dedicated to organizing and hosting long-term programs (7-8 weeks) and PhD schools (2-3 weeks) to foster breakthroughs in the fundamental understanding of the universe

Proposal for a **training program** in Quantum Information Theory, Quantum Computation and Communication, Theoretical Aspects of Quantum Technologies dedicated to **PhD students** to create a **bridge between theory and technology** at the first stage of their research ⇩

today's theoretical physics is tomorrow's technology innovation

The goal will be twofold: to get in touch the European and American theory community students and to allow them to gather with students coming from the quantum technology field, offering a unique opportunity to take advantage from the different expertise

We propose **two GGI Summer Schools** in July 2021 and in July 2022

—The first one (July 2021) will be focused on basic topics (**on-line** due to the COVID pandemic)

— The second one (July 2022) will be focused on advanced topics (**in person**). The training will follow the lines of the GGI Schools: lectures at the blackboard video-recorded and available in real time on the dedicated YouTube channel, desk and research facilities for students (https://www.ggi.infn.it/schools.html)

Slide material from Stefania De Curtis (INFN Florence)

Qubit encoding

- Quantum state and operator: nucleons (fermions) → qubits
- General mapping: Jordan-Wigner, or Bravyi-Kitaev
- A=2 dynamical particles ⇒ dimension 16, should require only 4 qubits.
  - First quantized mapping
  - Two qubits per particle to store lattice location

$$|1\rangle \equiv |\downarrow\downarrow\rangle \quad |2\rangle \equiv |\downarrow\uparrow\rangle \quad |3\rangle \equiv |\uparrow\downarrow\rangle \quad |4\rangle \equiv |\uparrow\uparrow\rangle$$

- Efficiency: *A* nucleons on *M* lattice sites with N_f fermion modes per site:
  - JW, BK: $N_f * M$ qubits (Hilbert space dimension = 2^{N_f*M})
  - Lattice location: $A \log_2 M$ qubits

A. Roggero et al, https://link.aps.org/doi/10.1103/PhysRevD.101.074038