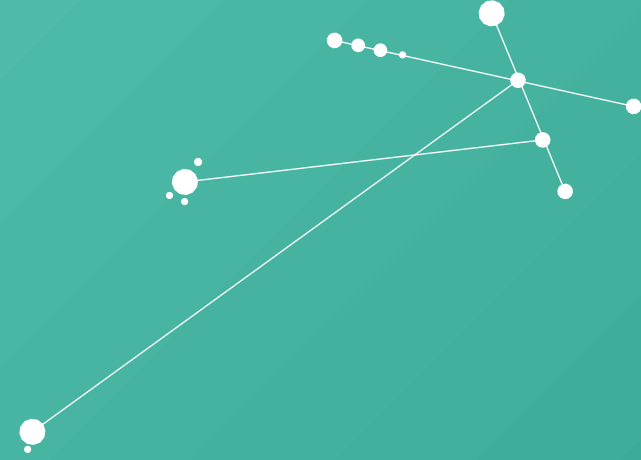


What Should Quantum Supercomputers Compute? From Quantum-Native Algorithms to Scientific Discovery –and Back

Harry Buhrman
PPD-NQCC seminar
23 September 2026



Technology, Scientific Discovery, and Commercialization



Scientific Discovery Precedes Industrial Advantage

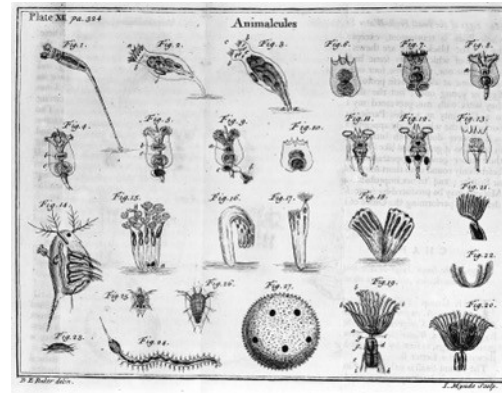
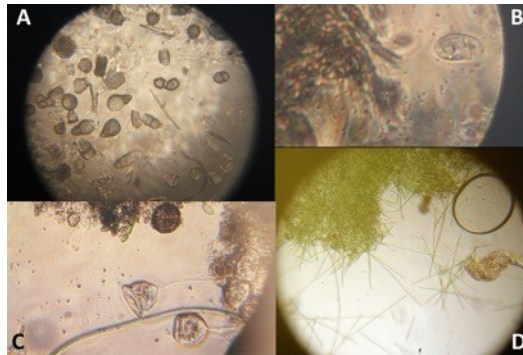
An example: microscope of **Antonie van Leeuwenhoek**



1674

- Built a 300 times better microscope
- Examine drops of water from a pond

Could see what nobody had seen before



Scientific Discovery Precedes Industrial Advantage

An example: microscope of **Antonie van Leeuwenhoek**



1674

- Built a 300 times better microscope
- Examine drops of water from a pond

Could see what nobody had seen before



Big Surprise & Discovery

- **Animalcules**: micro-organisms
- Bacteria, Protozoa, Algae etc.
- Birth of **microbiology**

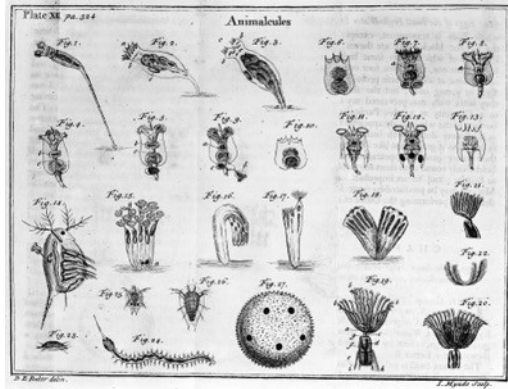
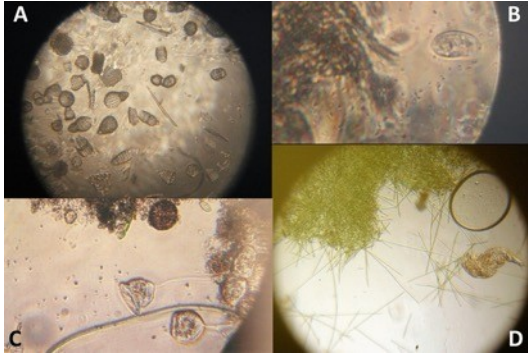
Industrial Advantage

- Unlocked advances in:
- Medicine, Agriculture, Food Production, Biotechnology, etc.

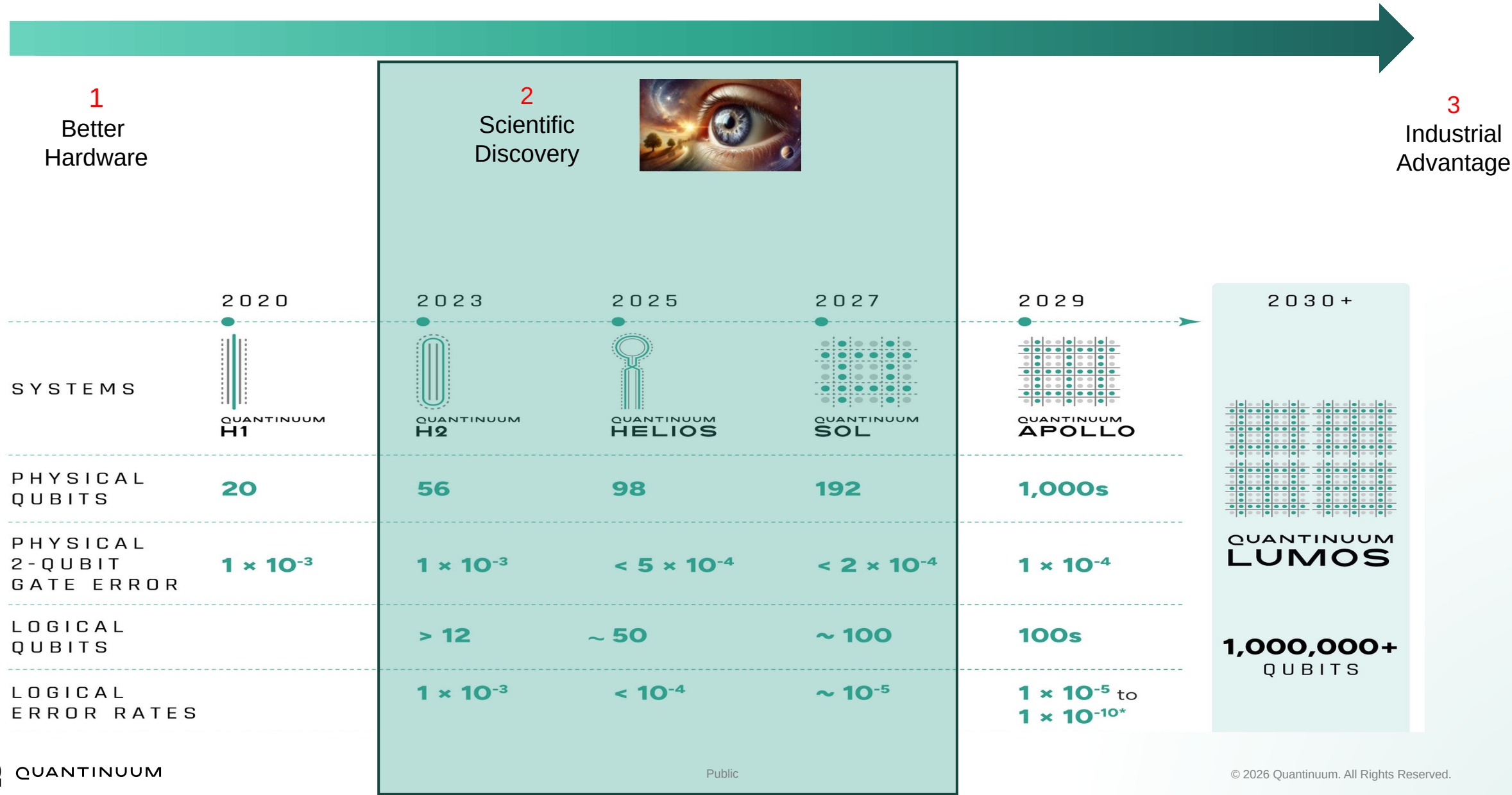
1
Better
Equipment/
Hardware

2
Scientific
Discovery

3
Industrial
Advantage



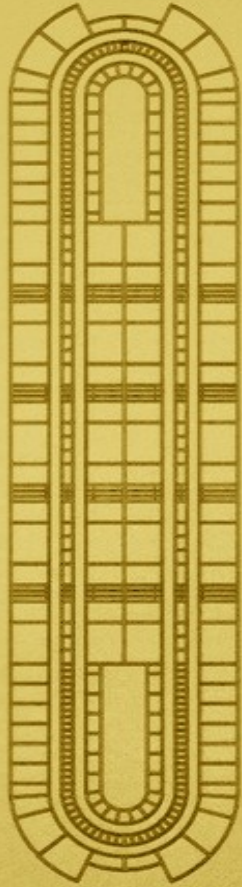
Scientific Discovery Precedes Industrial Advantage



Quantinuum

Quantum Charge-Coupled Device (QCCD)

- Low error: $< 10^{-3}$
- All-to-all connectivity
- Qubit reuse
- Mid-circuit measurement
- Gate Streaming





QUANTINUUM
HELIOS

Powered by Honeywell

Where Limits End and **Possibilities Dawn**

Helios continues to advance the state-of-the-art:

98 identical qubits

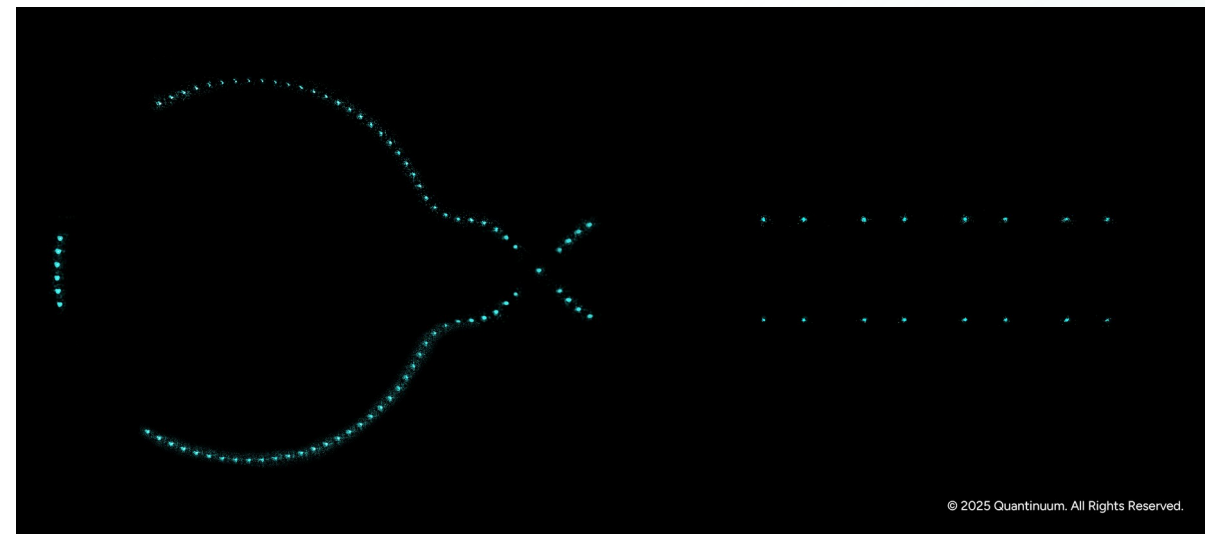
50 logical qubits*

99.92% two-qubit gate fidelity

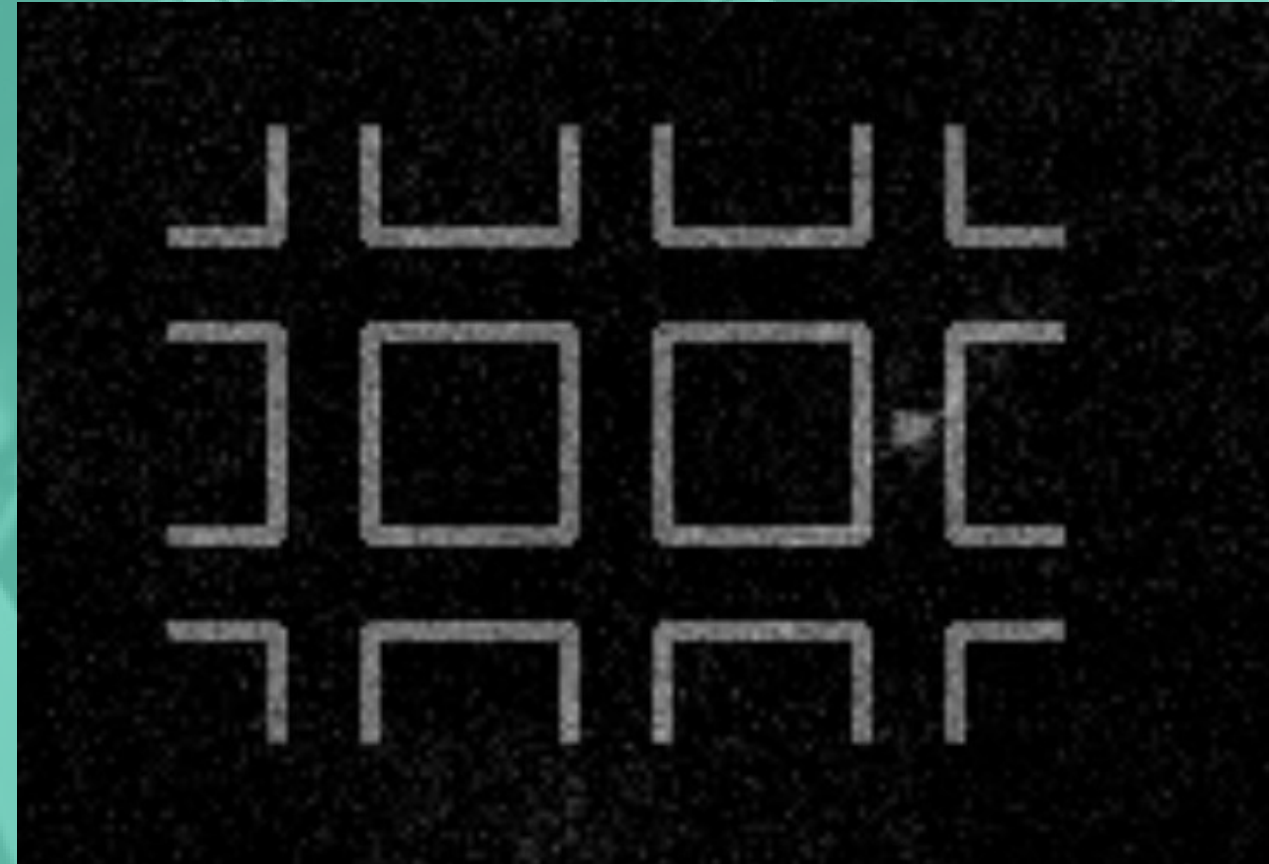
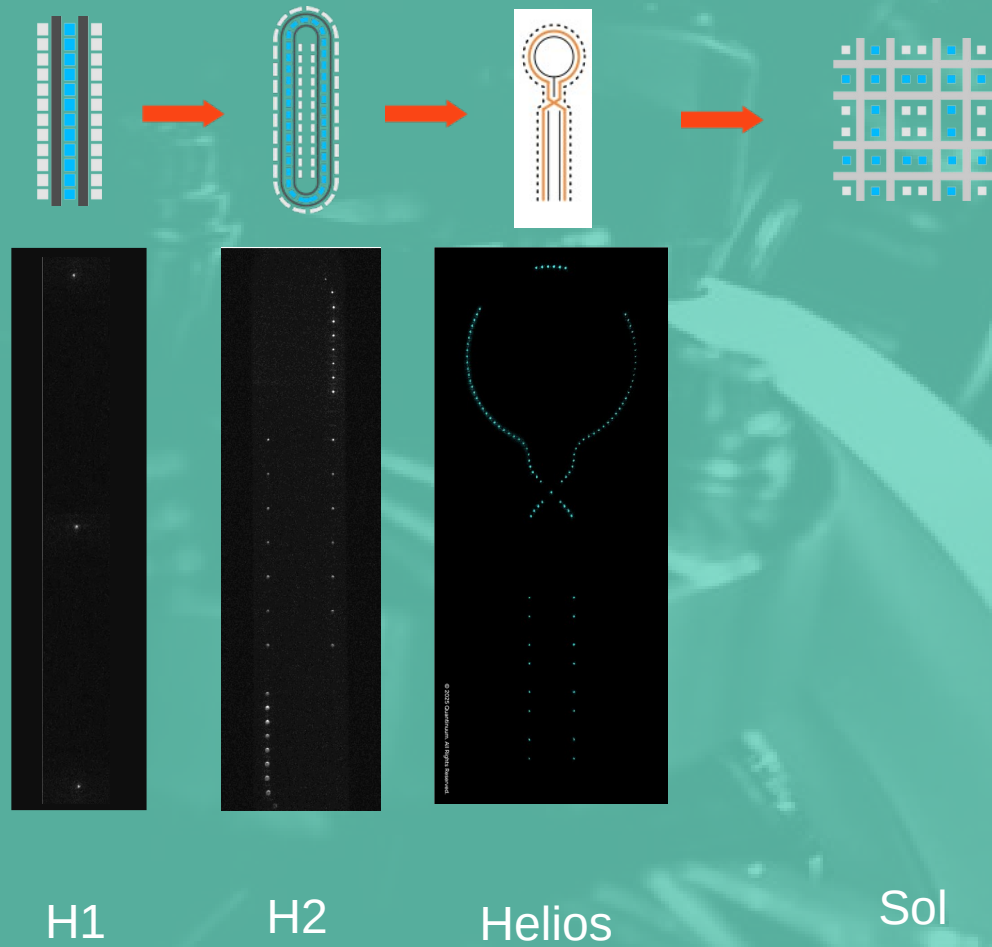
Faster circuit time with new chip design

Lower resources required per qubit

A single fully-dense depth-1 circuit on Helios

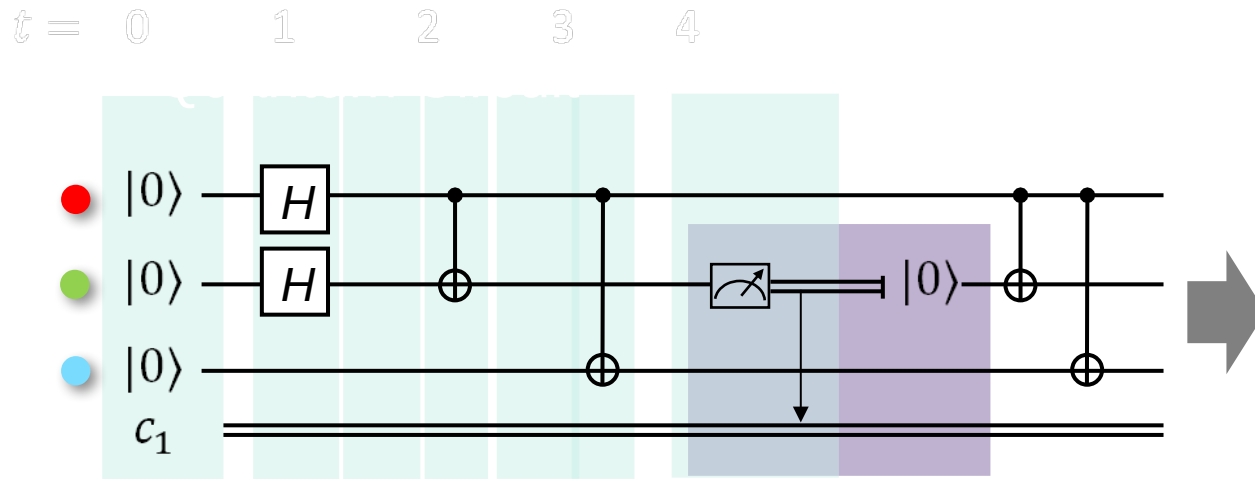


Trap Scaling Progress

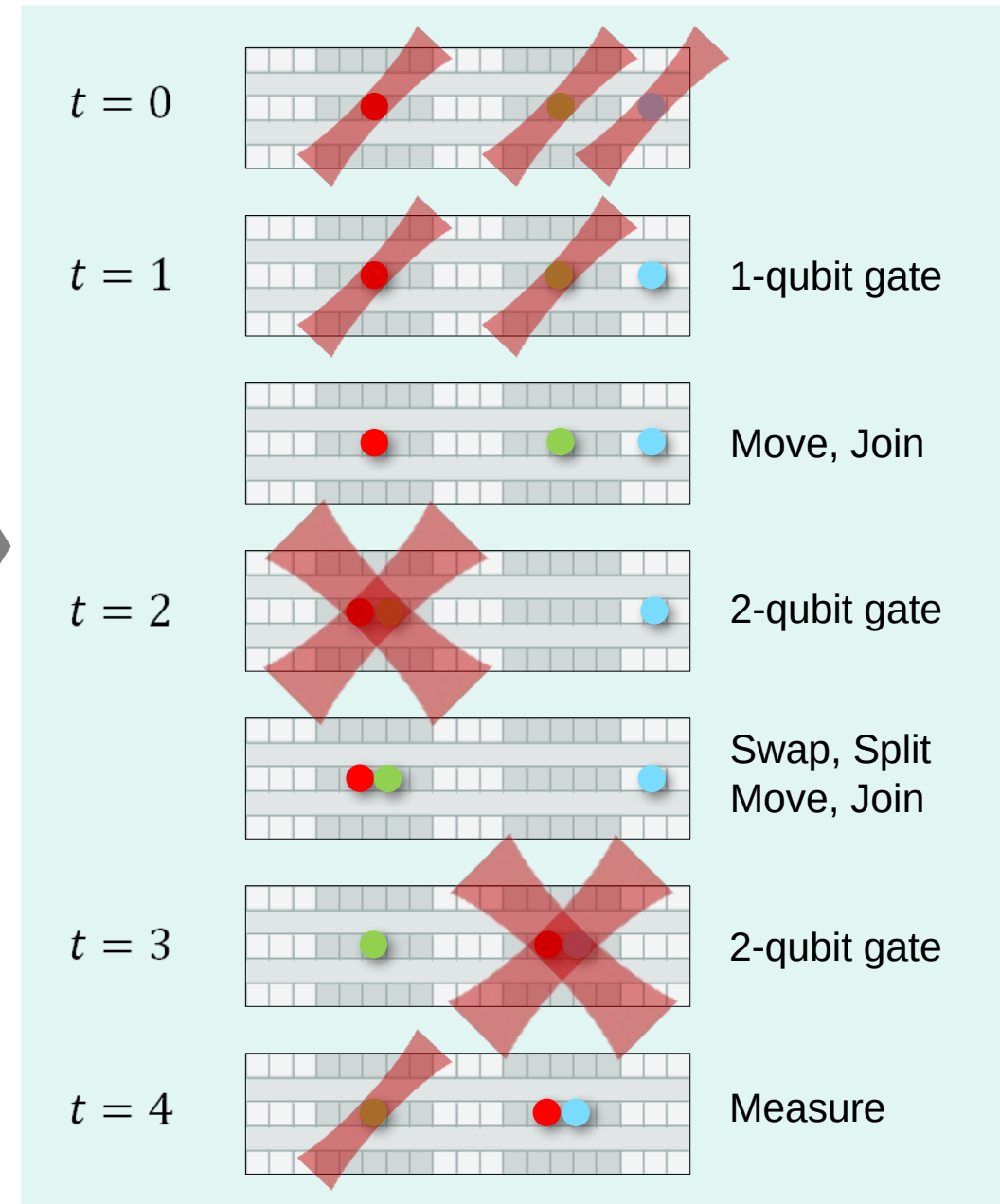


Grid-trap prototype

Physical Implementation



- No pre-defined “neighbor” qubits
- Operation fidelities are characterized by zones
- Control software tracks location of qubits



From Worst Case to Typical Instance!



Quantum Heuristics

- Worst case analysis is too stringent: hardest instance determines complexity
 - Focus on typical instances.
 - Develop quantum algorithms that are fast on typical instances but may be slow on others.
- Practice
 - We need a quantum computer to try them out!
 - Hardware is becoming more and more suitable!
- Theory
 - We need a theory to reason about (quantum) heuristics

- Definition a *Queasy* instance for a computational problem A:
 - *Quantum Easy*: fast quantum algorithm solves it
 - Classical algorithms struggle, feel *Queasy*
 - Formal definition in terms of *Instance Complexity & Kolmogorov complexity*

Formal Framework for Quantum Advantage

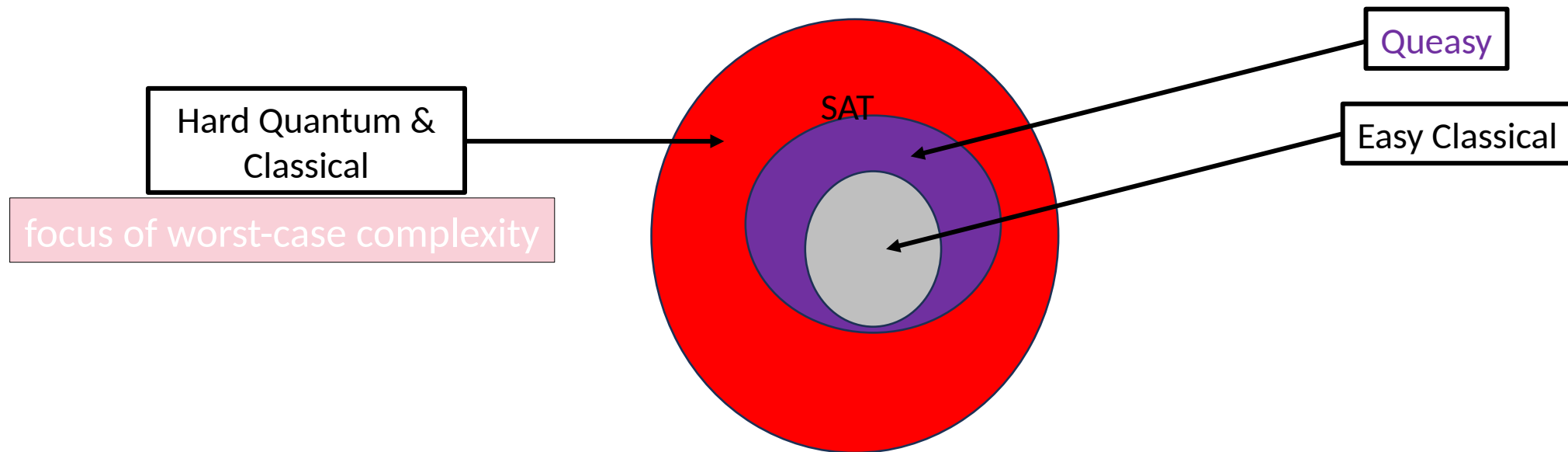
Harry Buhrman, Niklas Galke, Konstantinos Meichanetzidis

Quantinuum, Partnership House, Carlisle Place, London SW1P 1BX, United Kingdom

(Dated: October 3, 2025)

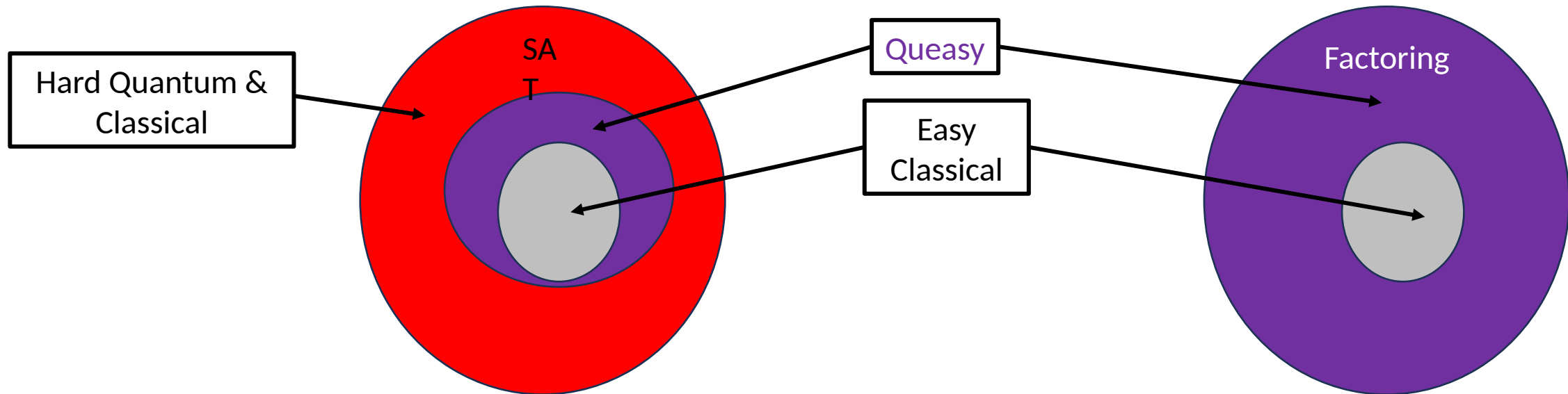
Queasy Instances

- Definition a *Queasy* instance is an instance of a comp. problem A:
 - *Quantum Easy*: fast quantum algorithm solves it
 - Classical algorithms struggle, feel *Queasy*
 - Formal definition in terms of *Instance Complexity & Kolmogorov complexity*
- Intuition: for SAT



Hunting for Queasy Instances

- Definition a *Queasy* instance is an instance of a comp. problem P:
 - *Quantum Easy*: fast quantum algorithm solve it
 - Classical algorithms struggle: feel *Queasy*
 - Formal definition in terms of instance complexity
- Intuition: for SAT and Factoring





What can you do with this new hardware?

What Should Quantum Supercomputers Compute?

Two routes to quantum advantage and useful scientific applications

BOTTOM-UP · QUANTUM-NATIVE

Start with a distinct quantum capability

- 01 Discover a quantum-native primitive
- 02 Resource estimates and validate on hardware
- 03 Identify use-case(s)

EXAMPLES

Complement sampling

Quantum Topological Data Analysis

Interacting-electron dynamics

use AI whenever and wherever you can!

TOP-DOWN · USE-CASE FIRST

Start with a scientific result/use-case worth achieving

- 01 Start with existing use-case
- 02 Resource estimates end-to-end workflow
- 03 Validate on hardware

EXAMPLES

Materials design

Quantum chemistry

Optimization, Drug design, etc.

use AI whenever and wherever you can!

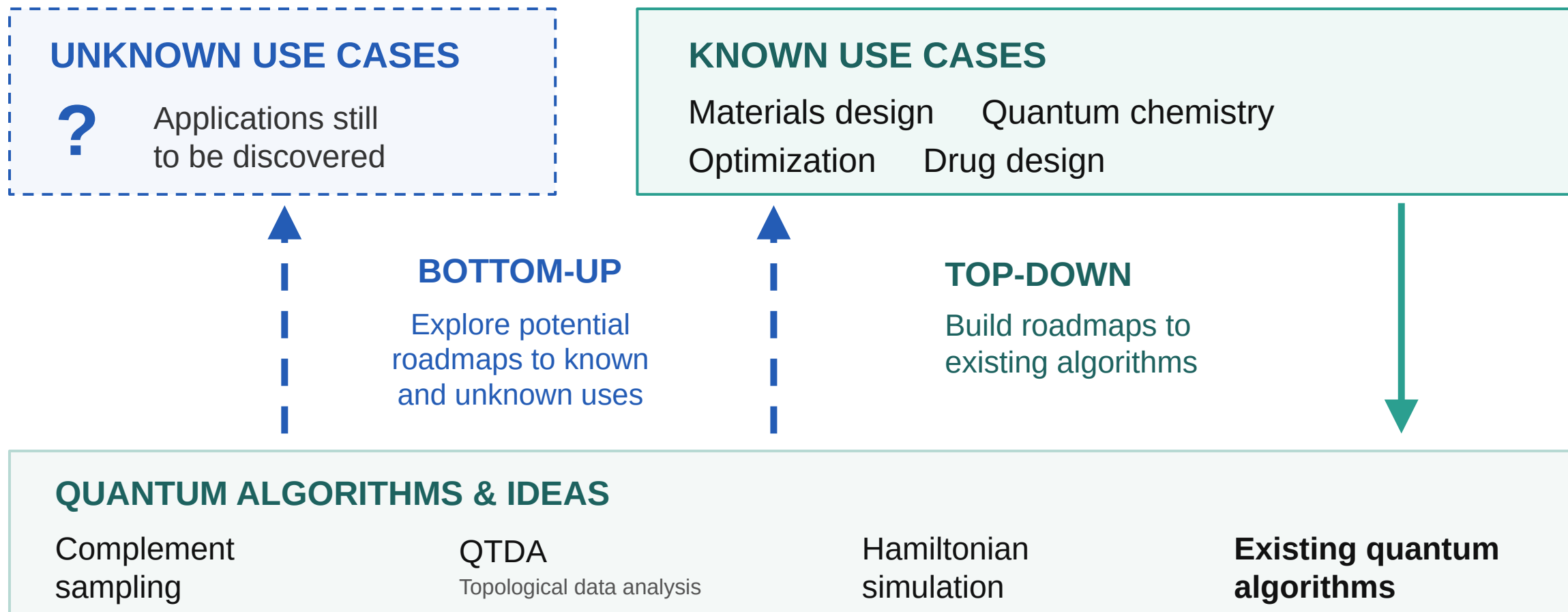
interplay



Hunting for *queasy* instances!!

Two Routes to Useful Quantum Applications

Known problems guide algorithms. Quantum ideas can reveal new applications.



AI can help develop and connect both routes

Complement Sampling

PHYSICAL REVIEW LETTERS **136**, 040601 (2026)

Editors' Suggestion

Provable and Verifiable Quantum Advantage in Sample Complexity

Marcello Benedetti^{1,*}, Harry Buhrman^{1,2,3,†} and Jordi Weggemans^{2,4,‡}

¹*Quantinuum, London, United Kingdom*

²*QuSoft, Amsterdam, The Netherlands*

³*University of Amsterdam, Amsterdam, The Netherlands*

⁴*CWI, Amsterdam, The Netherlands*



(Received 11 August 2025; revised 20 October 2025; accepted 9 December 2025; published 27 January 2026)

Setting: sample-to-sample complexity

- Given samples from distribution D_1 , output a **single** (classical) sample from a distribution D_2 (w.h.p)
- Example: given uniformly random bits, generate samples from some distribution of interest D
- comparing # **quantum** samples versus # **classical** samples needed

Quantum samples

Given a distribution $D : S \subseteq [N] \rightarrow [0,1]$, a quantum sample is a single copy of the state

$$|S_D\rangle = \sum_{x \in S} \sqrt{D(x)} |x\rangle$$

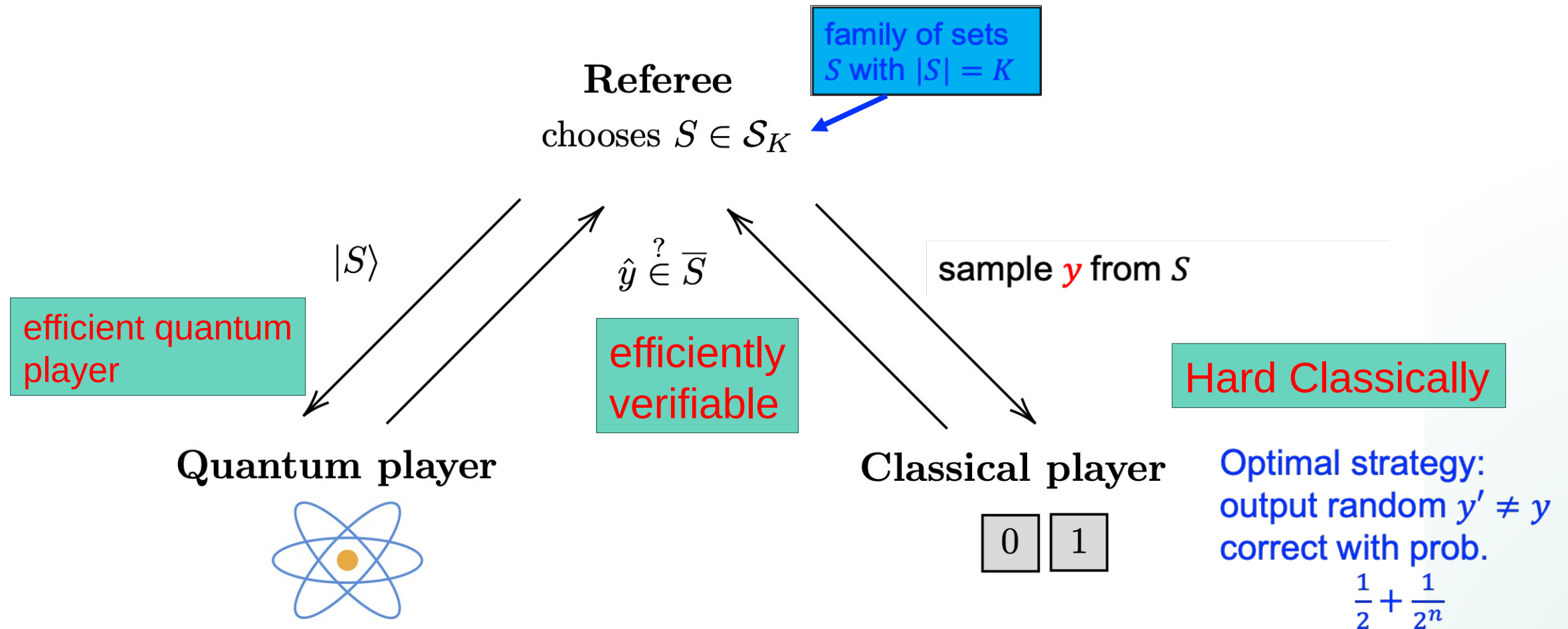
If D is the uniform distribution, we write $|S\rangle$.

The task: complement sampling

$$|S\rangle = \frac{1}{\sqrt{|S|}} \sum_{x \in S} |x\rangle$$

Let $N = 2^n$, $S \subseteq [N]$ with $|S| = K = N/2$.

Task: given samples from S , provide a (uniformly random) sample from $\bar{S} = [N] \setminus S$.

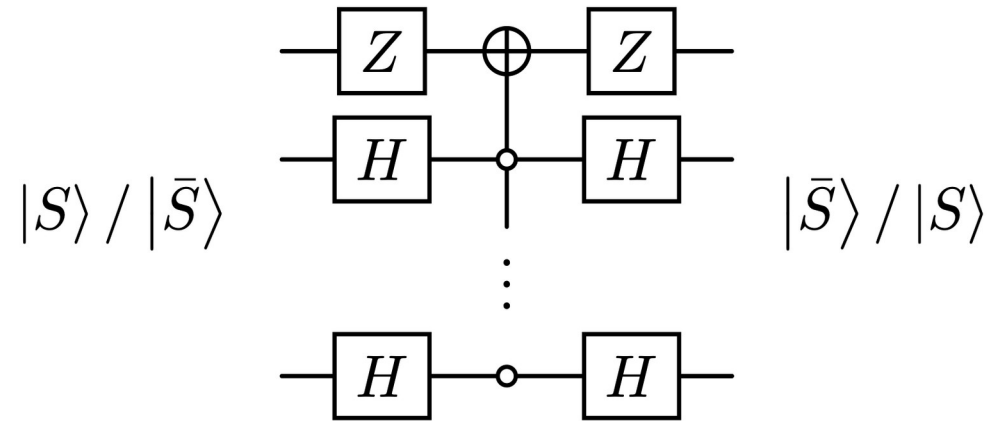


The efficient quantum sampler

$$|S\rangle = \frac{1}{\sqrt{|S|}} \sum_{x \in S} |x\rangle$$

Get $|S\rangle$, apply the swapping circuit to obtain $|\bar{S}\rangle$ and measure in the computational basis

$$|S\rangle = \frac{1}{\sqrt{|S|}} \sum_{x \in S} |x\rangle$$

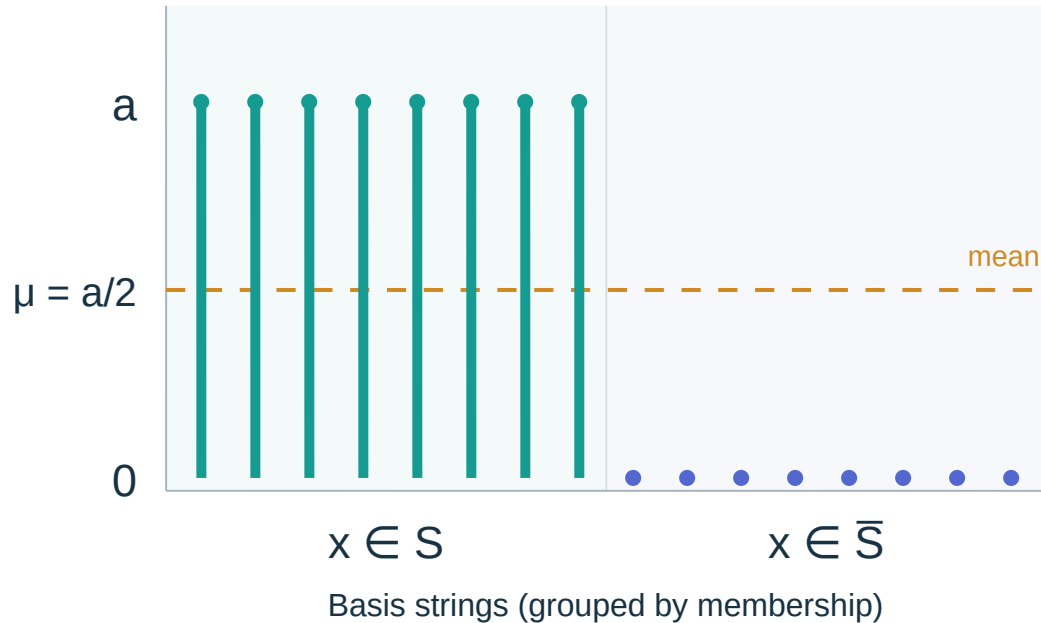


Note: uses a universal gate set

Quantum complement swapper as Grover diffusion

$$N = 2^n, \quad |S| = |\bar{S}| = N/2, \quad a = 1/\sqrt{(2^{n-1})}, \quad \mu = a/2$$

Before: $|S\rangle$

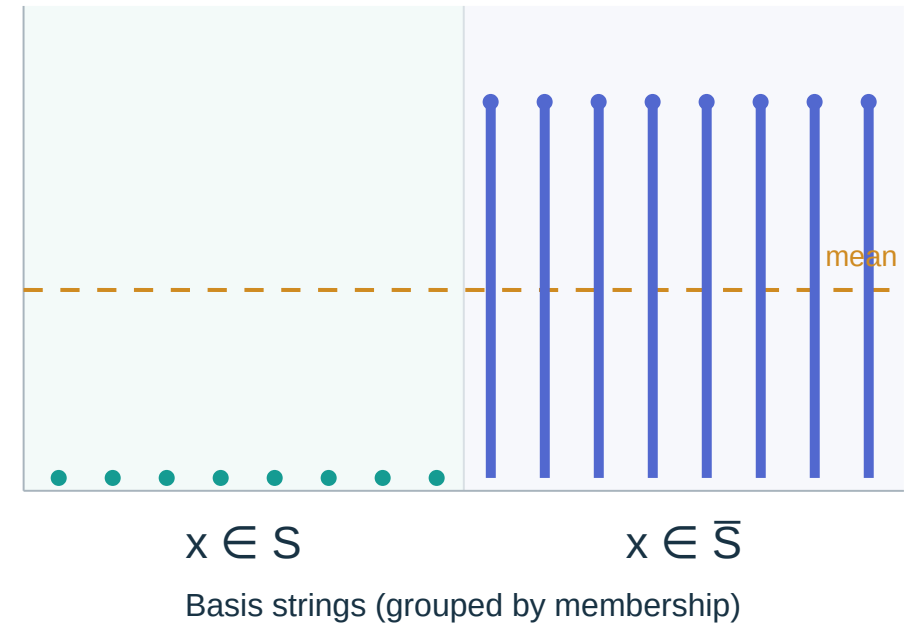


$$x \in S: a \mapsto 2(a/2) - a = 0$$

After: $|\bar{S}\rangle$

Grover diffusion

$$\alpha_x \mapsto 2\mu - \alpha_x$$



$$x \in \bar{S}: 0 \mapsto 2(a/2) - 0 = a$$

$$D = 2|+\rangle \otimes^n \langle +| \otimes^n - I \quad D|S\rangle = |\bar{S}\rangle$$

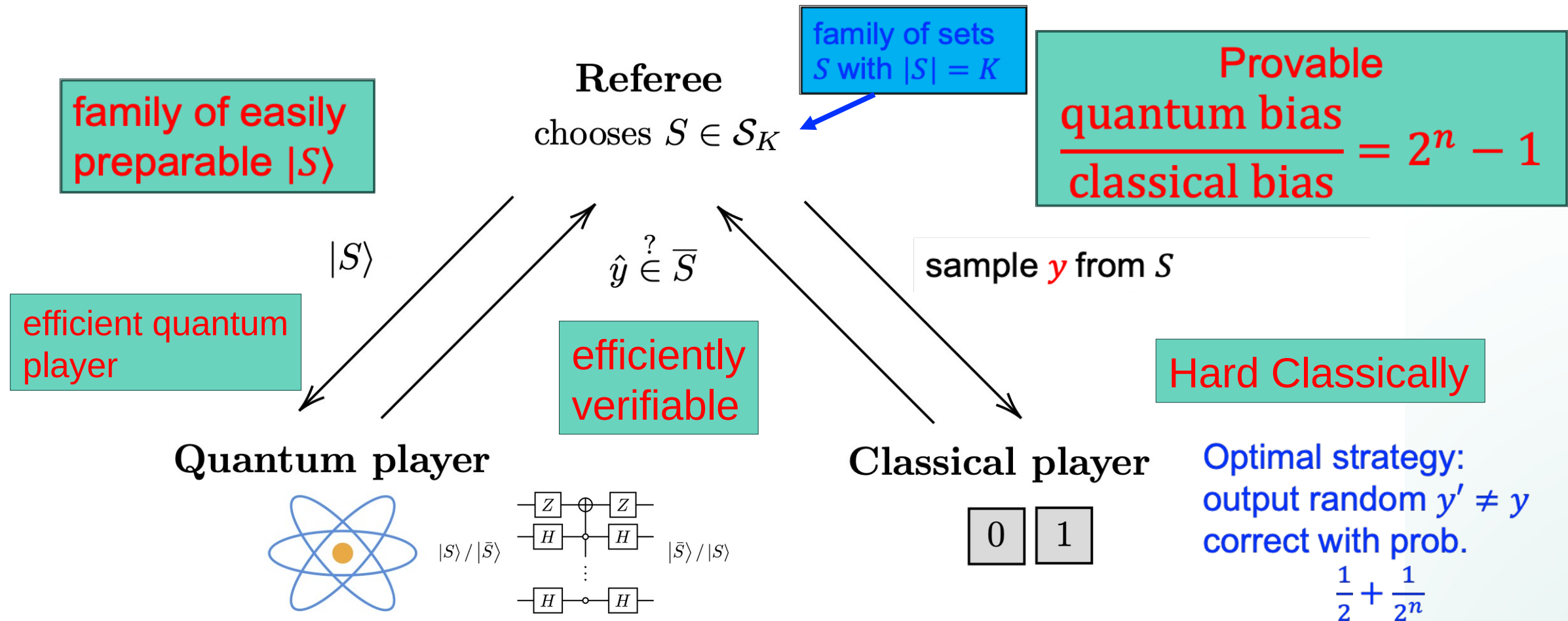
One reflection swaps the occupied and empty halves. No membership oracle is needed.

The task: complement sampling

$$|S\rangle = \frac{1}{\sqrt{|S|}} \sum_{x \in S} |x\rangle$$

Let $N = 2^n$, $S \subseteq [N]$ with $|S| = N/2$.

Task: given samples from S , provide a (uniformly random) sample from $\bar{S} = [N] \setminus S$.



Experimental verification

Unconditional and exponentially large violation of classicality

Received: 11 June 2026

Accepted: 21 August 2026

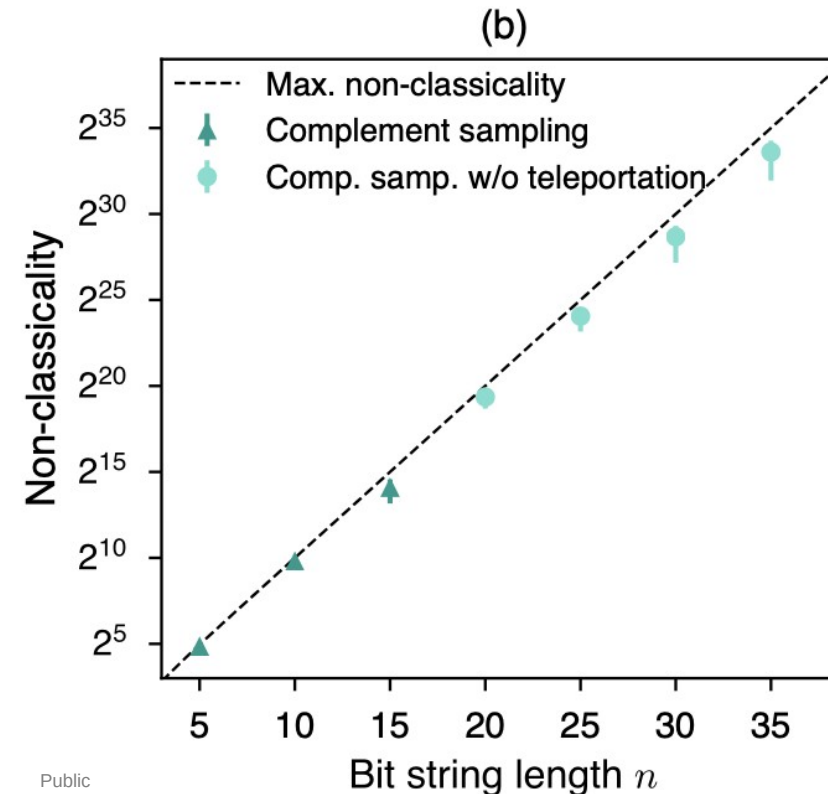
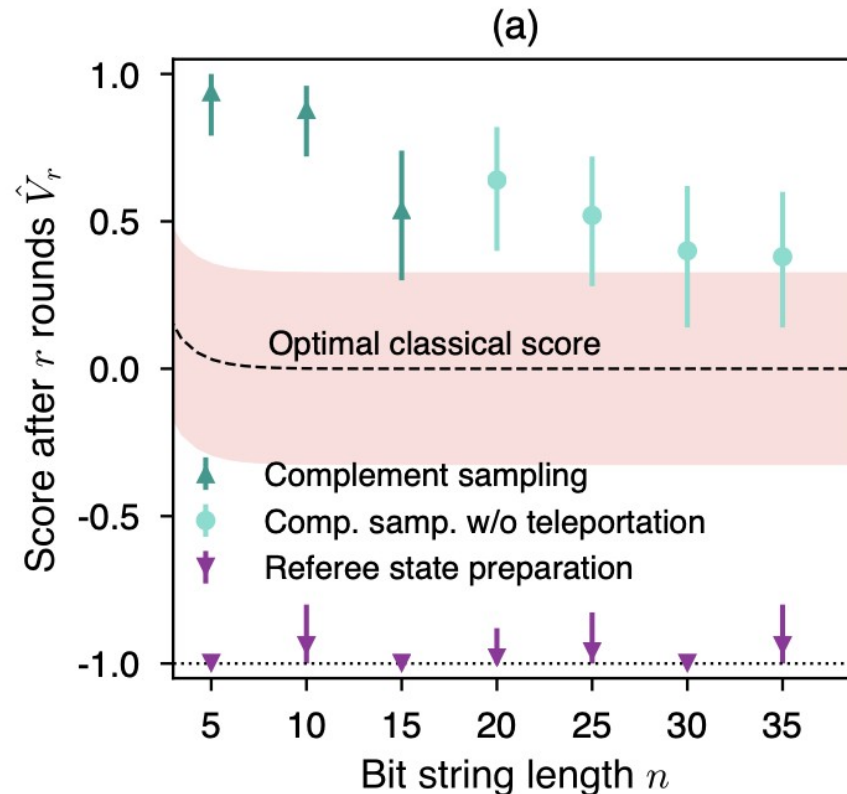
Published online: 05 September 2026

Marcello Benedetti¹✉, Gabriel Marin-Sanchez¹, Jordi Weggemans¹,
Matthias Rosenkranz¹ & Harry Buhrman^{1,2,3}✉

Exponential violation on H2 using 56 qubits

Good Benchmark

- Provable quant. adv. ($\approx 2^{35}$)
- Efficiently verifiable
- Scalable

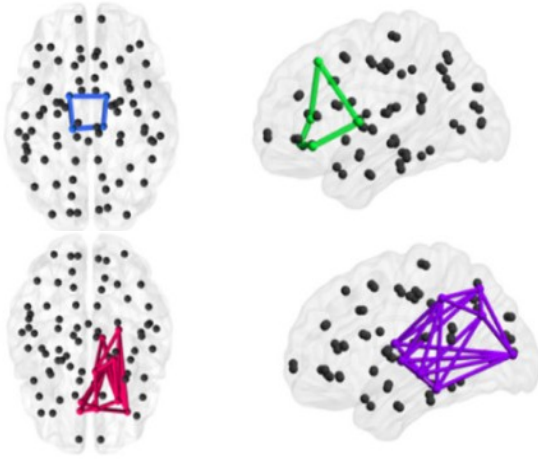




Quantum Topological Data Analysis

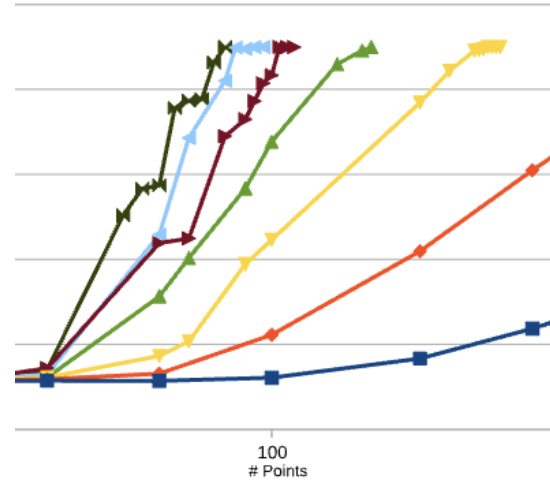
Team of Adam Connolly

Why are we doing this?



Highly-connected networks appear in many scientific domains, but their high-dimensional structure is poorly understood

Memory Limits for PH based on Homology Dimension



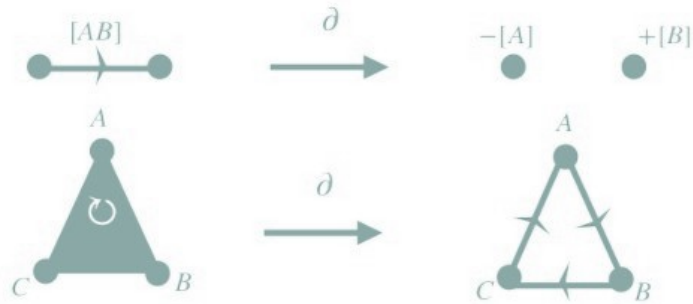
Classical methods have **limitations in practice**:

- Graph neural networks (GNNs) miss global features
- Topological data analysis (TDA) packages struggle in high dimension

Goal:

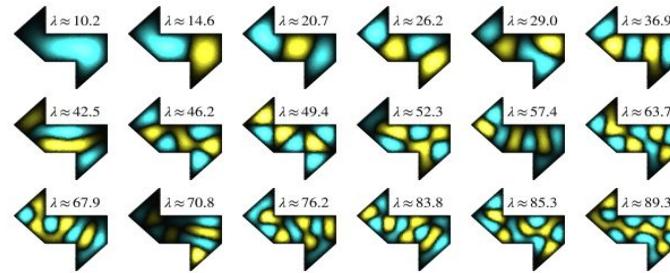
- Utility-scale QCs promise to extract **classically inaccessible** features from dense, highly-connected networks
- Use quantum-generated features for downstream tasks: anomaly detection, network analysis, classification, ML pipelines

Quantum advantage in analyzing the Laplacian



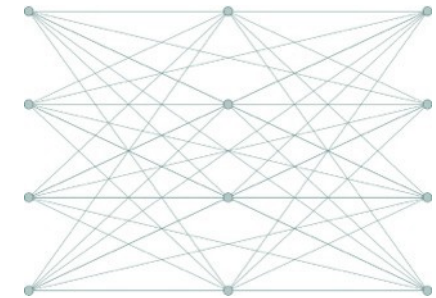
The **Laplacian_k** matrix encodes **k-partied interactions**

It generalizes **heat flow** to k-partied **information flow**



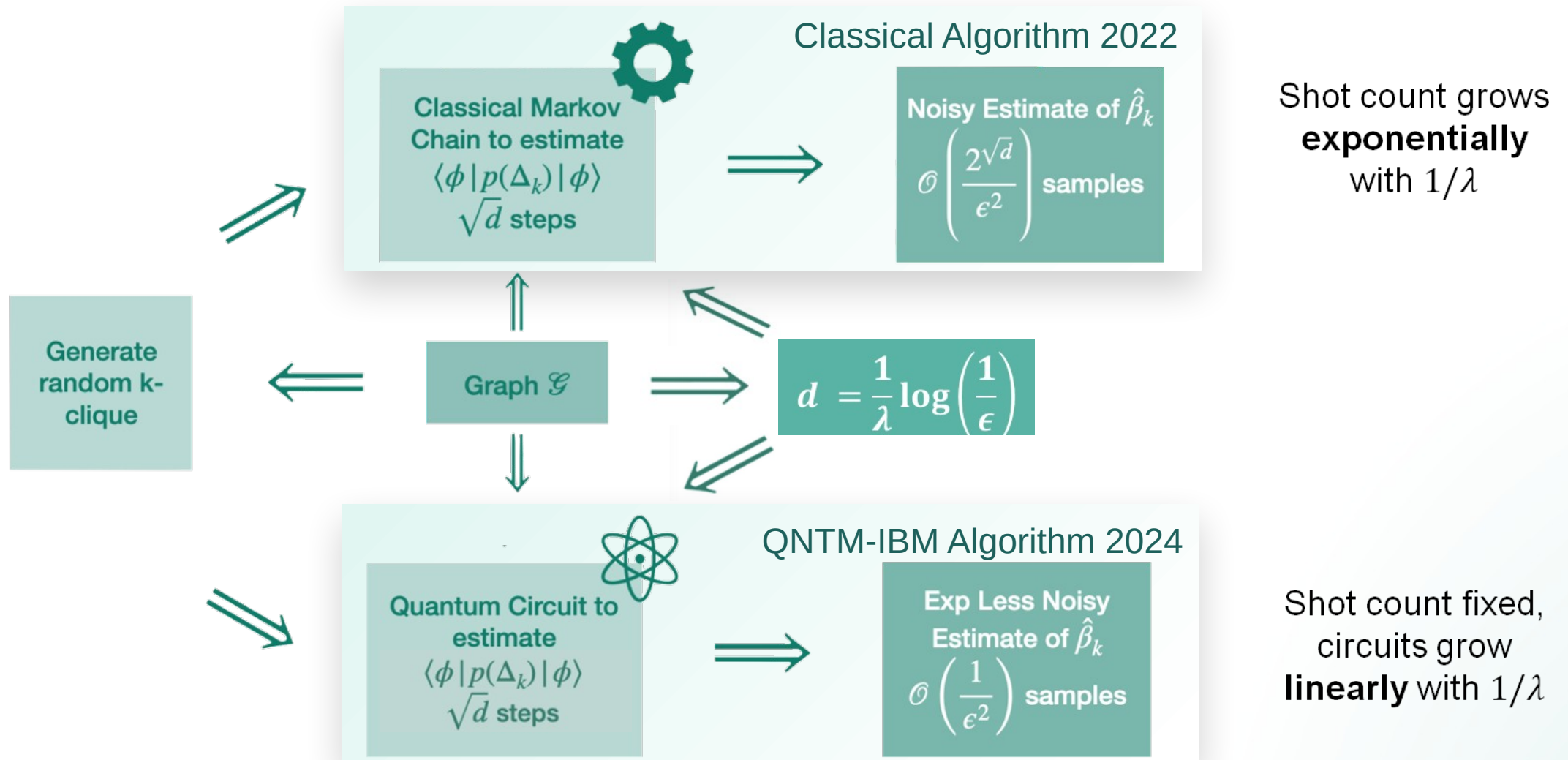
The Laplacian captures the **modes of flow**, including:

- Betti number (holes)
- Eigengap (mixing time)
- Rate of communication



Size of the Laplacian **grows exponentially with k** but can be encoded in **quantum circuit with $O(n^2)$ gates**

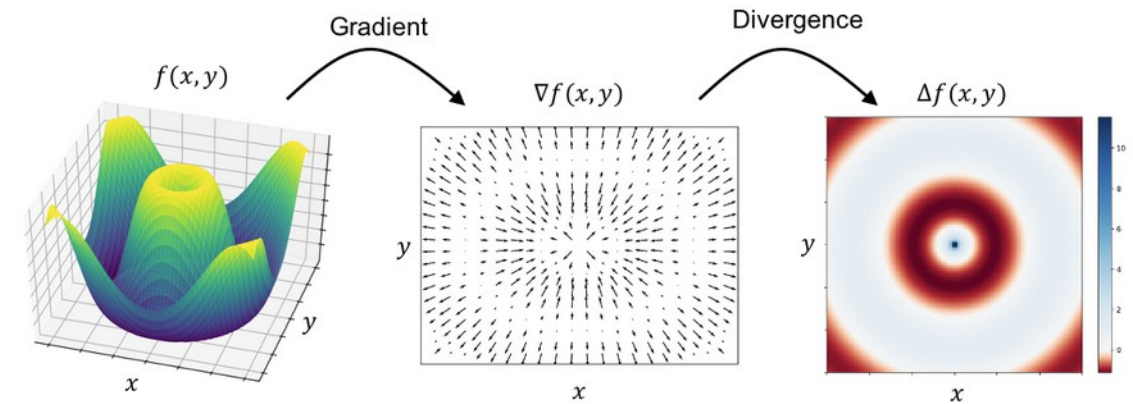
Structure of Classical and Quantum Algorithms



Topological Quantum Analysis of Networks (ToQAN)

Laplacian moments

- Beyond normalized Betti numbers
- Independent "**geometric**" value, describe diffusion on graphs
- Potential **exponential** quantum speed-up
- Classical simulation through **CoLE** package



Source: <https://www.frontiersin.org/journals/computational-neuroscience/articles/10.3389/fncom.2013.00189/full>

ToQAN pipeline

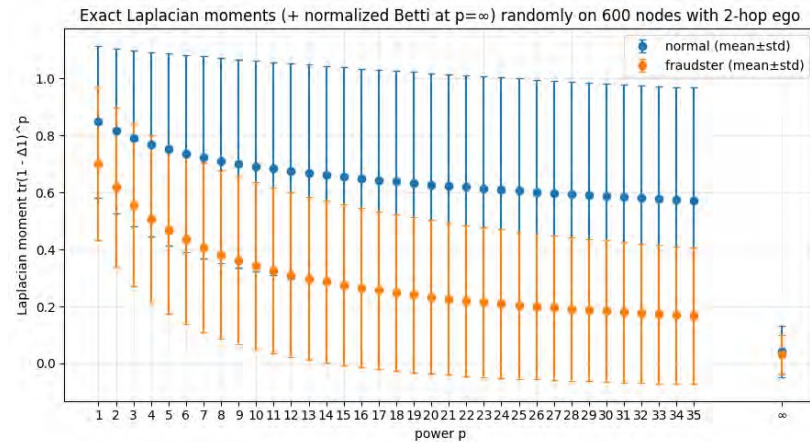
- Generate egonets from graph data
- Detect higher-order structures via **CoLE**
- Compute Laplacian-based features
- Augment graph features
- Train and evaluate ML models

ToQAN API

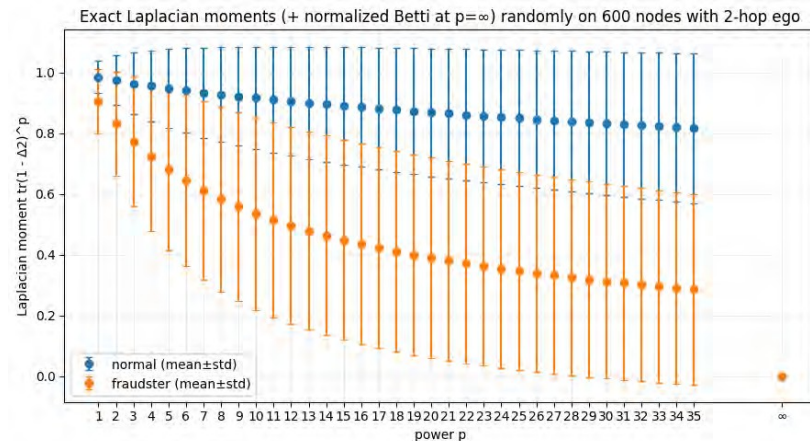
- Provides egonet-generation utilities
- Exposes Laplacian-metric computation services
- Supports graph-feature augmentation
- Interfaces with standard ML architectures
- Enables model training and evaluation
- Supports checkpointing and CoLE extensions

ToQAN use case: Fraud detection with Softbank

First-order Laplacian moment

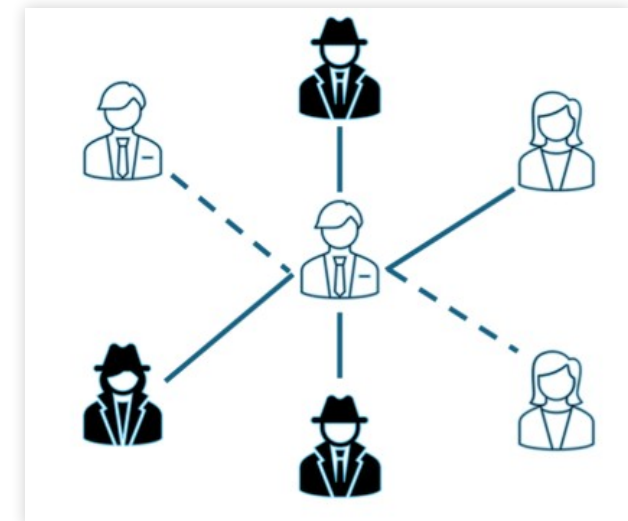


Second-order Laplacian moment



[Recent white paper with Softbank: Telecommunications fraud detection](#)

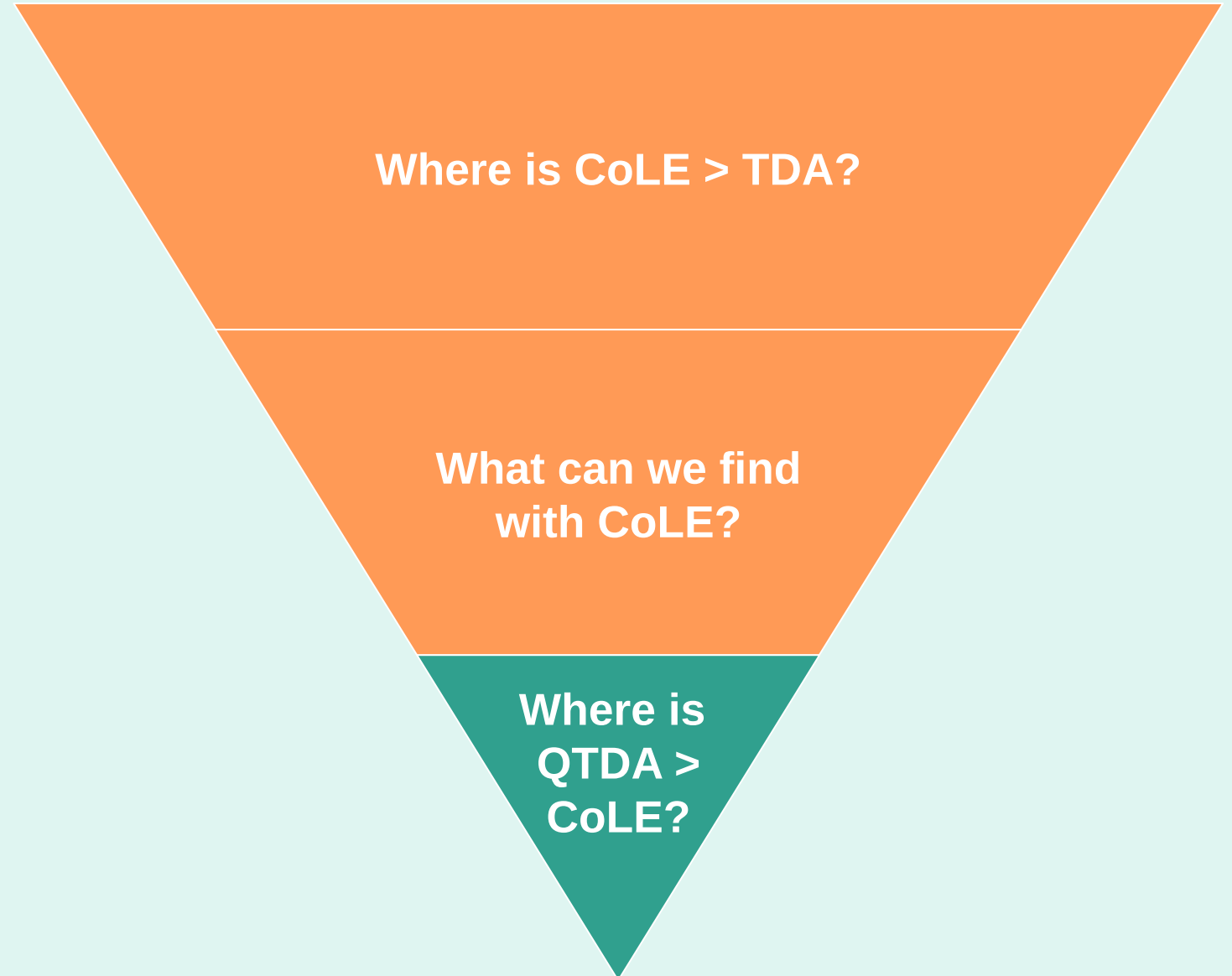
- Telephone-call graph representation
- Egonet extraction from first- and second-hop neighborhoods
- Laplacian-based topological feature generation
- GNN training on structural and node features
- Fraud prediction on unlabeled networks



Source: <https://open-evidence.com/2024/12/16/mapping-geometry-fraud-machine-learning-science/>

Telecommunications fraud detection

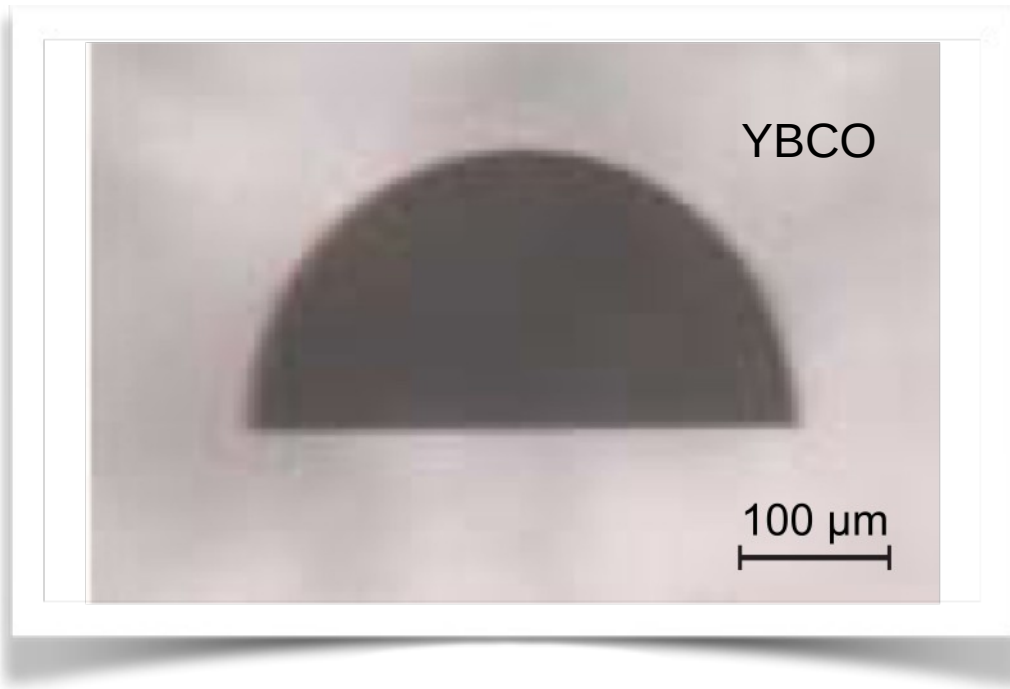
- Improvements by including Laplacian moment information
- Low-order moments were sufficient, but still **efficiently accessible with CoLE**
- Explore other graph data (e.g. transactional) with potential to **show higher-order relationships**



Simulation of Physics

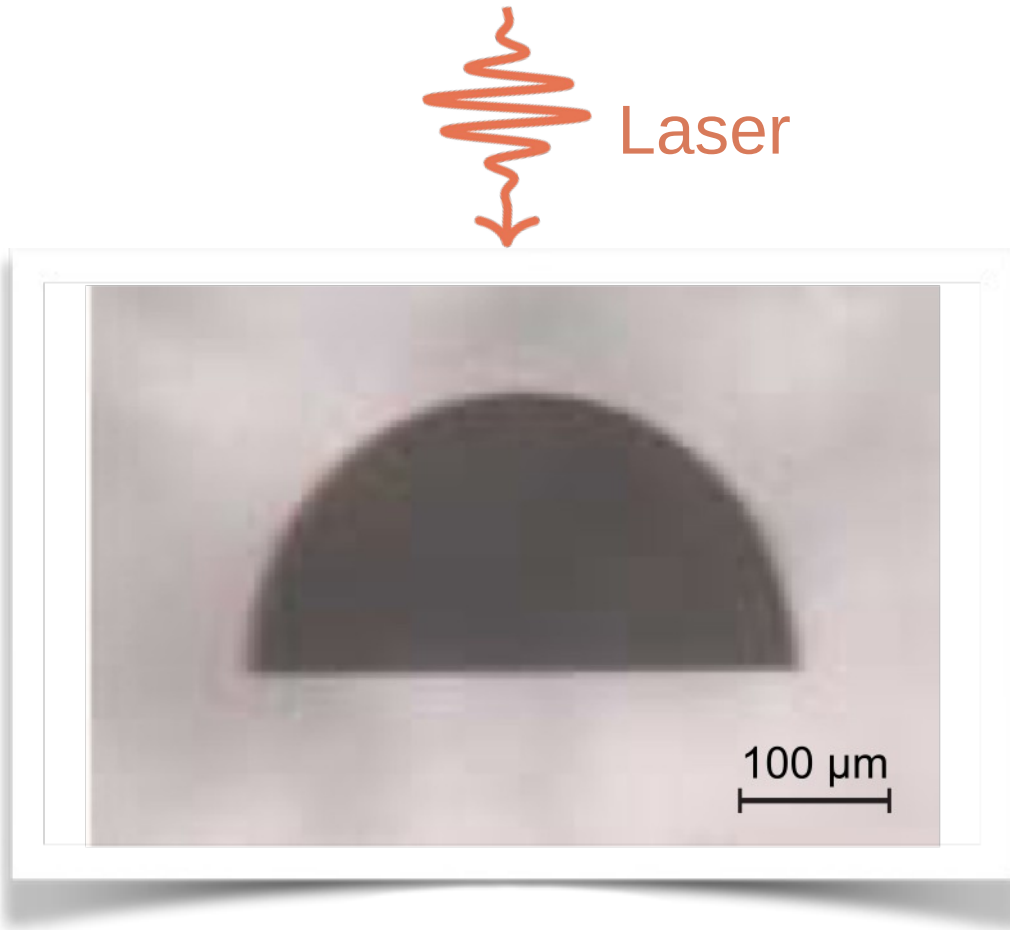
Team of Henrik Dreyer

High-temperature superconductors

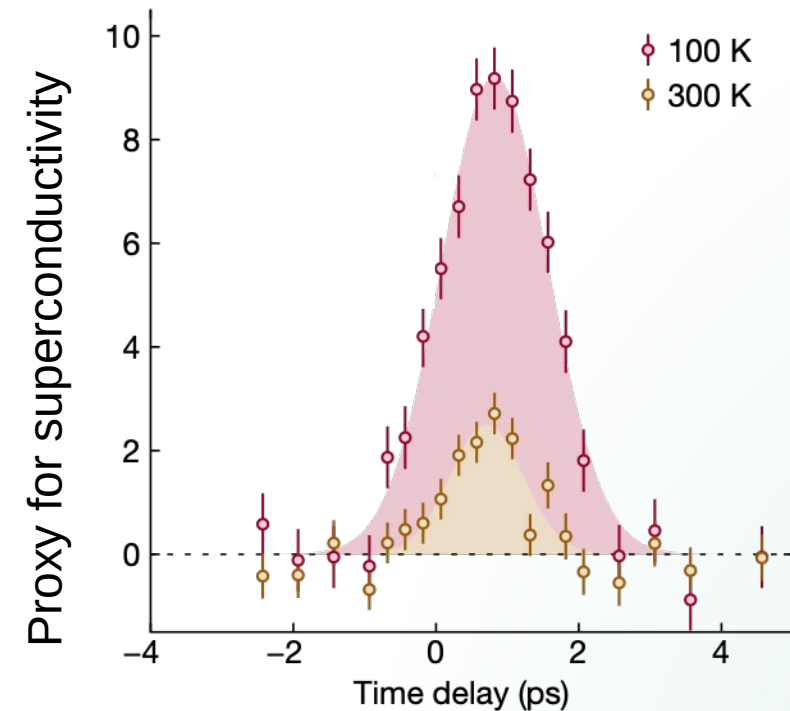


- High-temperature superconductors are produced by many companies and sold on to end users in nuclear fusion, nuclear magnetic resonance, motors & generators — any time large magnet fields are required

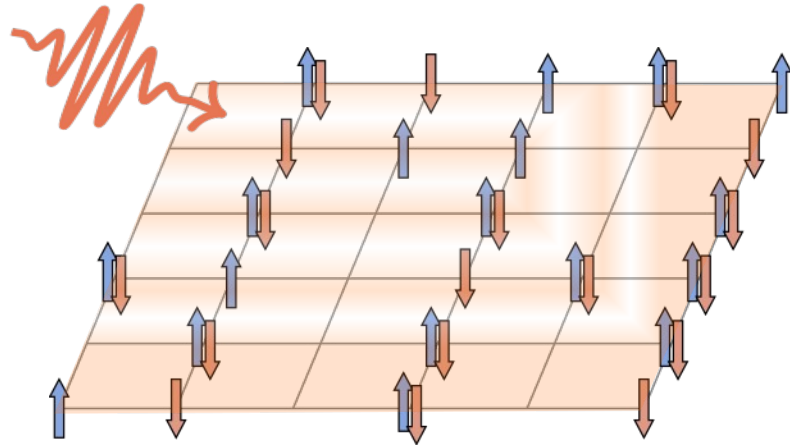
High-temperature superconductors



- Recently, signatures of superconductivity were observed at room temperature (300 Kelvin), after irradiating Yttrium Barium Copper Oxide with light.
- The superconductivity is only stable for a few picoseconds.



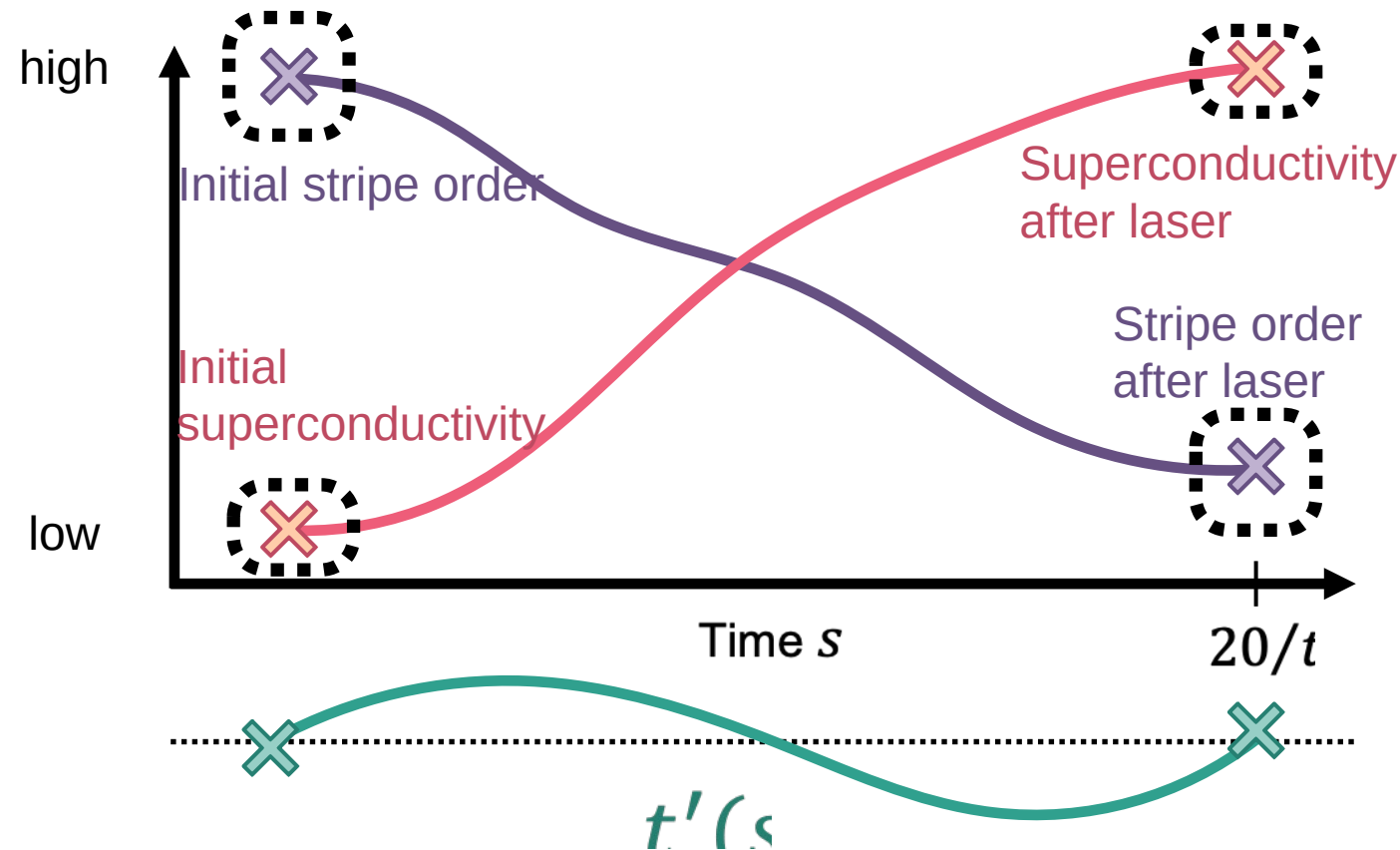
High-temperature superconductors



- Recently, signatures of superconductivity were observed at room temperature (300 Kelvin), after irradiating Yttrium Barium Copper Oxide with light.
- The superconductivity is only stable for a few picoseconds.
- There are many competing hypothesis for the mechanism behind this. If we can figure out which one is correct, we can use that knowledge to try and stabilize the state for longer times.
- One such hypothesis postulates that the superconductor is described by an extended Fermi-Hubbard model and that the laser destroys stripe ordering that competes with superconductivity.

High-temperature superconductors

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} - \boxed{t'(s)} \sum_{\langle\langle ij \rangle\rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma} +$$



- Testing these hypotheses is classically hard but straightforward to do with a quantum computer in principle:
 - Step 1: Prepare a room-temperature state of the extended Hubbard model.
 - Step 2: Simulate irradiation with a laser by tuning a parameter of the model (t').
 - Step 3: Measure both superconductivity and stripe order.

High-temperature superconductors

H

Superconducting pairing correlations on a trapped-ion quantum computer

Etienne Granet,¹ Sheng-Hsuan Lin,¹ Kevin Hémerly,¹ Reza Hagshenas,² Pablo Andres-Martinez,³ David T. Stephen,² Anthony Ransford,² Jake Arkinstall,³ M.S. Allman,² Pete Campora,² Samuel F. Cooper,² Robert D. Delaney,² Joan M. Dreiling,² Brian Estey,² Caroline Figgatt,² Cameron Foltz,² John P. Gaebler,² Alex Hall,² Ali Husain,⁴ Akhil Isanaka,² Colin J. Kennedy,² Nikhil Kotibhaskar,⁵ Michael Mills,² Alistair R. Milne,⁵ Annie J. Park,² Adam P. Reed,² Brian Neyenhuis,² Justin G. Bohnet,² Michael Foss-Feig,² Andrew C. Potter,² Ramil Nigmatullin,³ Mohsin Iqbal,¹ and Henrik Dreyer^{1,*}

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⁵*Quantinuum, Partnership House, Carlisle Place, London SW1P 1BX, UK*

(Dated: November 5, 2025)

Current J

macroscopic $\mathcal{O}(L) \rightarrow$ superconductor

Summary & Conclusions

- Scientific Discovery
 - Current quantum hardware: explore and discover phase
 - Commercial application will come a little bit later
- Quantum Heuristics
 - Worst case analysis is too limiting
 - Design quantum algorithms for typical instances
- Two Principles
 - Top down: use-case first (happens most often)
 - Bottom up: start with quantum native algorithm
 - Use AI whenever you can
- Examples
 - Complement Sampling, Quantum Topological Data Analysis, and Interacting-electron dynamics

Thank You