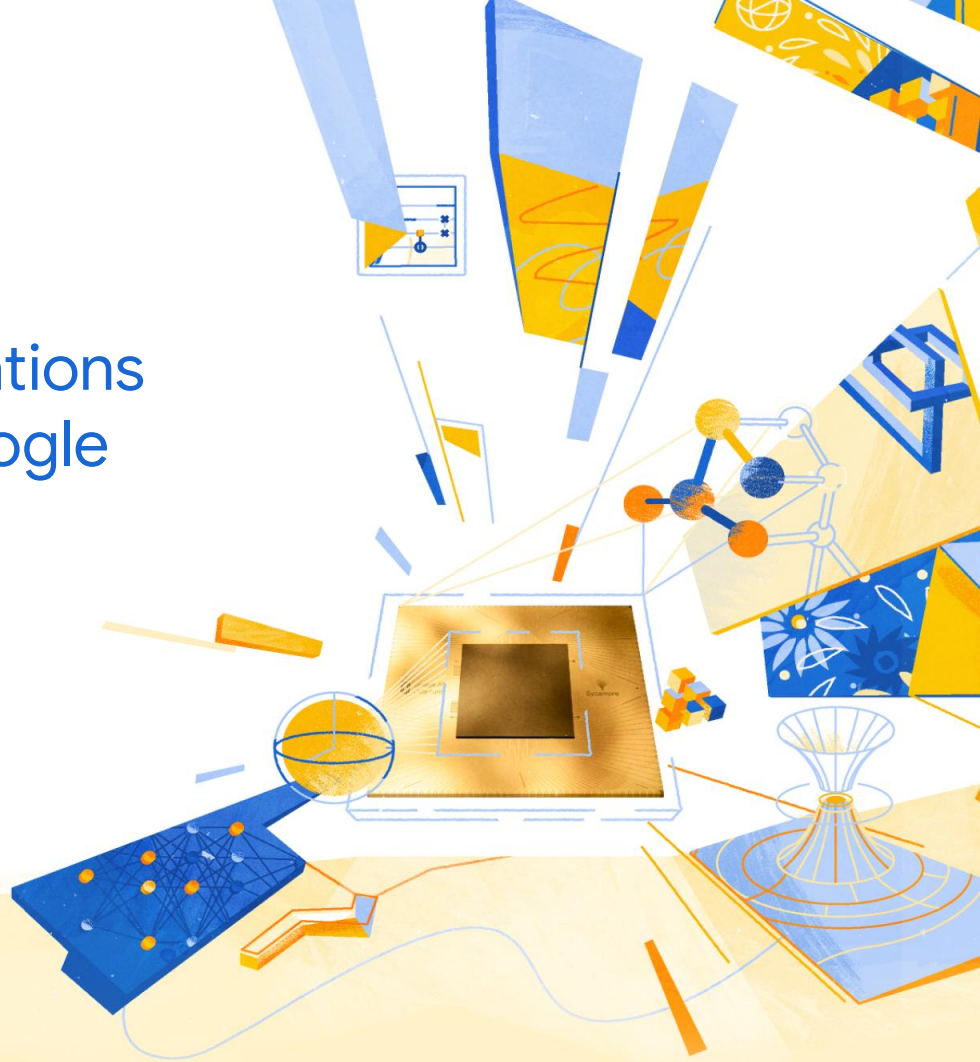




# Searching for valuable applications of quantum computing at Google

# Ryan Babbush

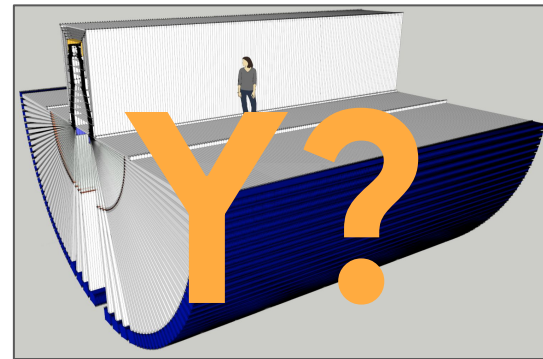
December 14, 2023



# Google is building an error-corrected quantum computer

Targeting a device with ~1M physical qubits  
that can execute billions, or trillions of gates

**This is a challenging and expensive endeavor!**



→ We hope these devices will solve important and otherwise intractable problems!

There are some use cases for 1M physical qubits, but fewer than we would hope

**This talk is about research into the viability of promising quantum applications**

# Outline

1. Brief discussion of Google's roadmap towards quantum error-correction
2. Review of fault-tolerant quantum algorithms for chemistry
3. Results on identifying and assessing viability of valuable chemical applications
4. The viability of quantum advantage in topological data analysis
5. Brief overview of some other interesting results and directions in applications



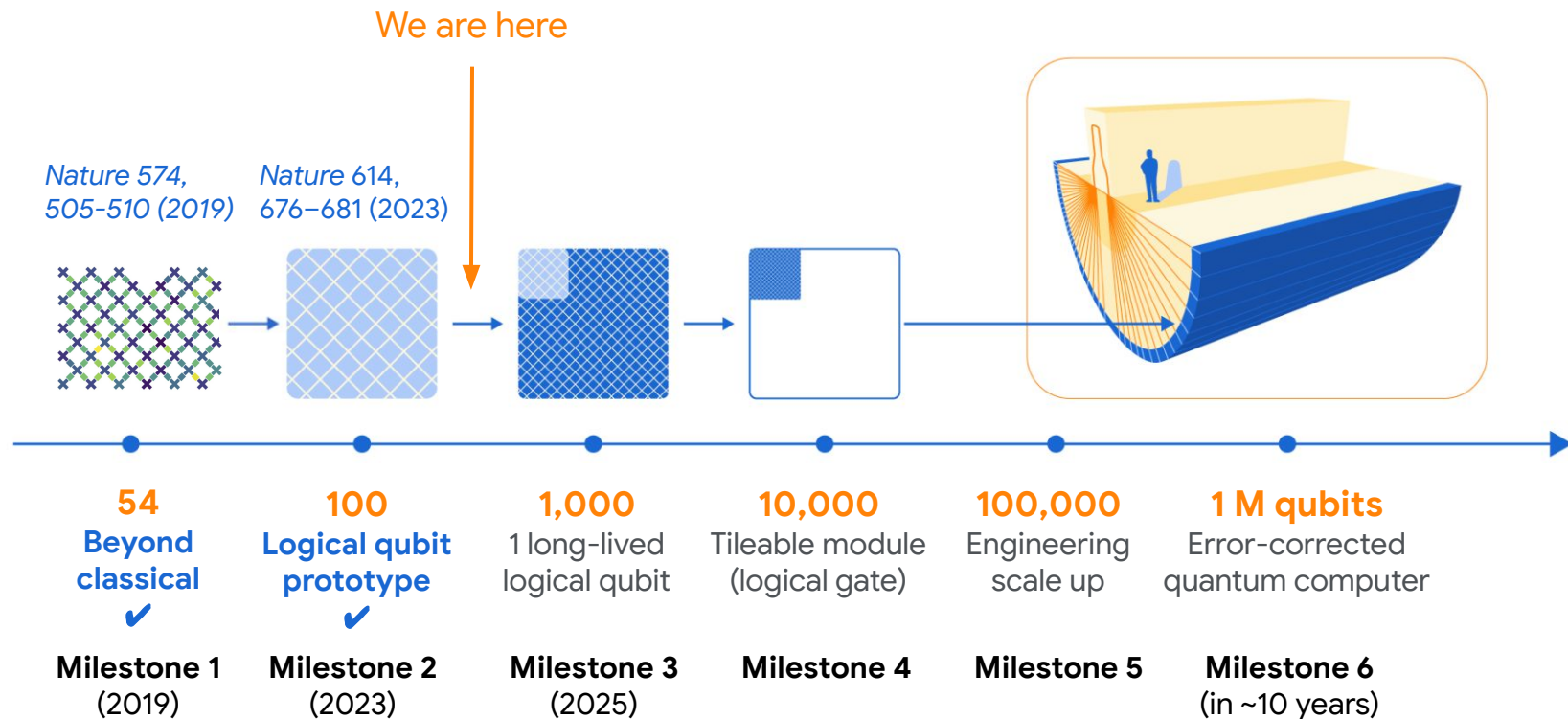


# Part I: Google's roadmap towards quantum error-correction



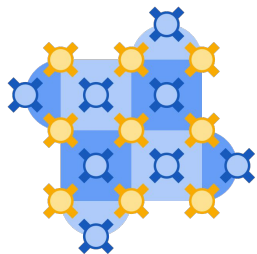


# Google's roadmap towards practical quantum computing

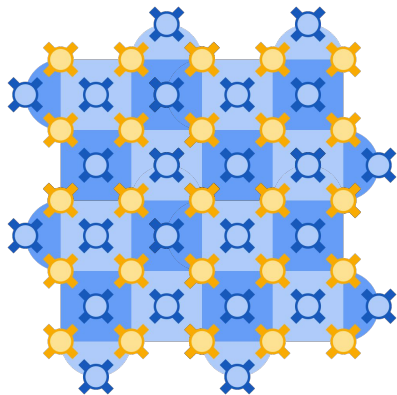


## Milestone 2: Logical qubit prototype (plan)

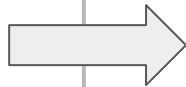
Run experiments to implement surface codes



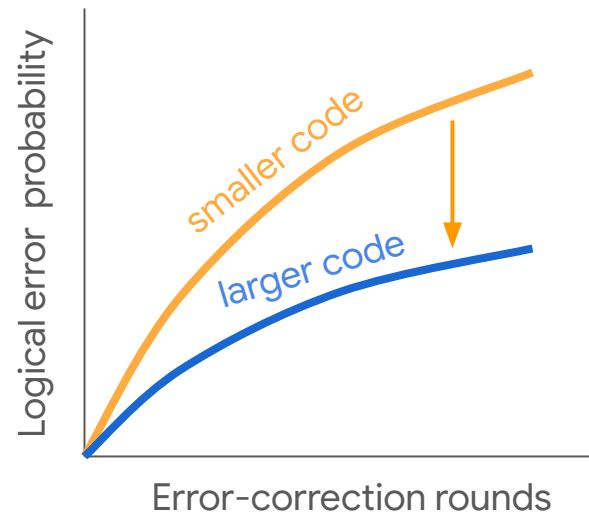
$d = 3$   
surface code



$d = 5$   
surface code

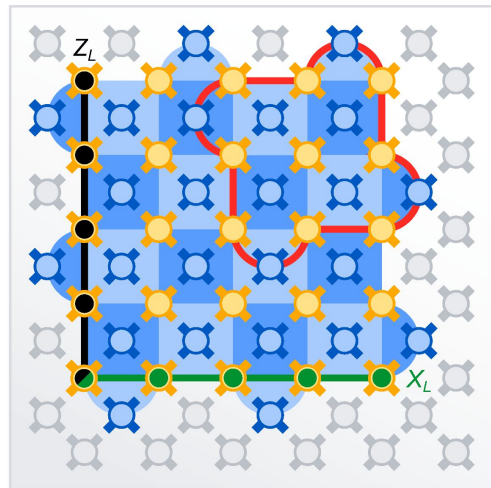






Analyze data and see if failure probability is lower with larger code

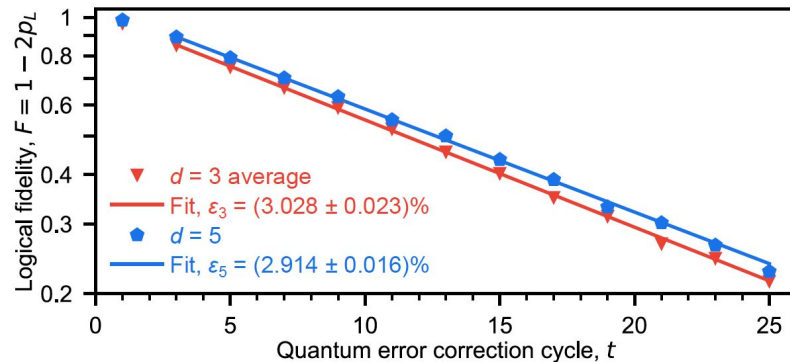


# Milestone 2: Logical qubit prototype (experimental data)

*Nature* 614, 676–681 (2023)



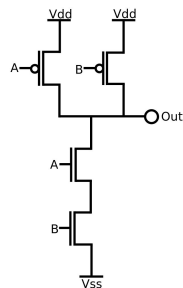
-  Data qubit ( $d^2$ )
-  Measure qubit ( $d^2 - 1$ )
-  Unused
-  Subset distance-3



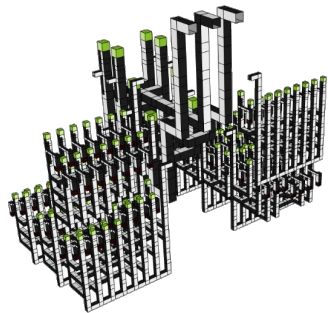
$$\lambda = \text{error}(d) / \text{error}(d + 2)$$

# On the importance of super-quadratic speedups

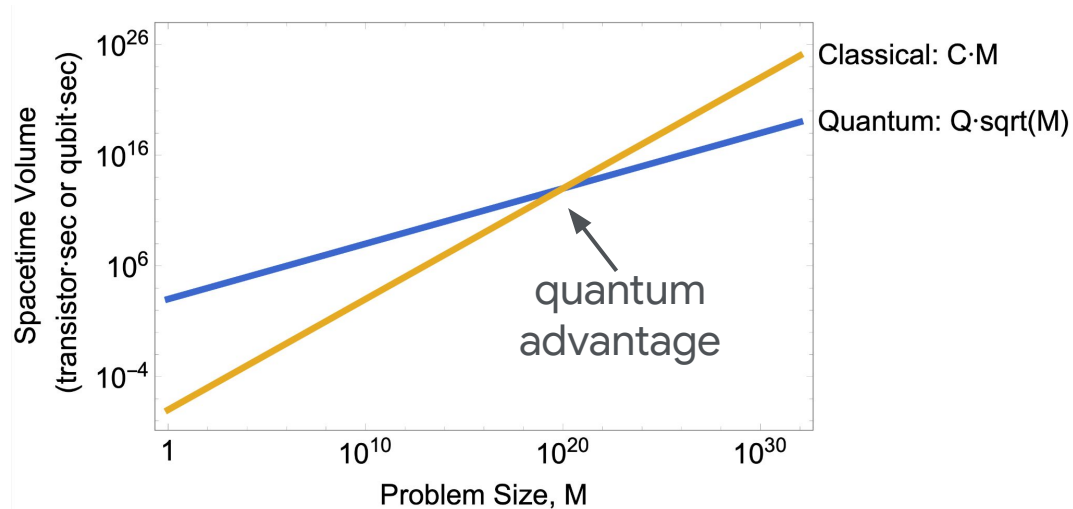
PRX Quantum 2, 010103 (2021)



classical NAND gate (CMOS)  
 $<10^{-9}$  “transistorseconds”



“quantum NAND” gate (distillation of Toffoli state)  $>10$  “qubitseconds”



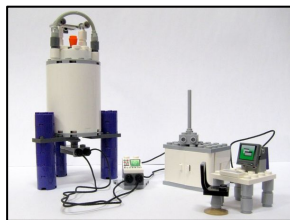
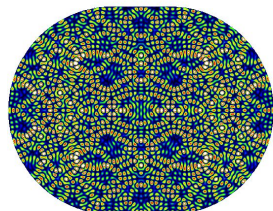
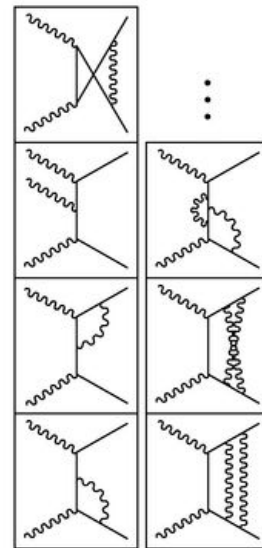
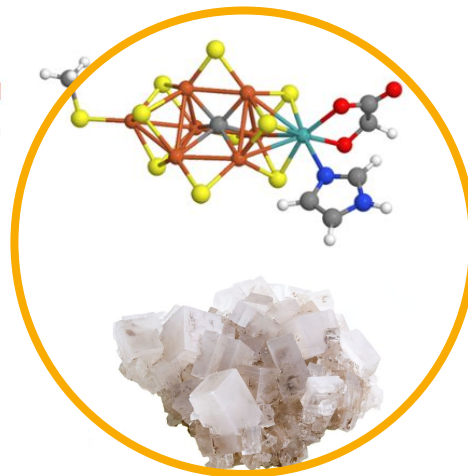
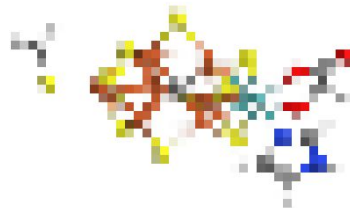
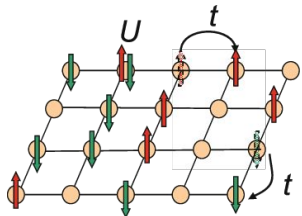
PRX Quantum 2, 010103 (2021) argues quadratic speedups will not enable error-corrected advantage until devices MUCH larger than 1MM physical qubits



## Part II: review of fault-tolerant quantum algorithms for chemistry



# Spectrum of quantum simulation difficulty



application difficulty



physical  
qubits  
required

25k-50k

50k - 250k

250k - 1MM

1MM - 5MM

???

# The molecular electronic structure problem

Solve for the energy of molecule under the Born-Oppenheimer approximation

$$H = \sum_{pq} (T_{pq} + U_{pq}) a_p^\dagger a_q + \sum_{pqrs} V_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

$$T_{pq} = \int dr \varphi_p^*(r) \left( -\frac{\nabla^2}{2} \right) \varphi_q(r)$$

$$U_{pq} = \int dr \varphi_p^*(r) U(r) \varphi_q(r)$$

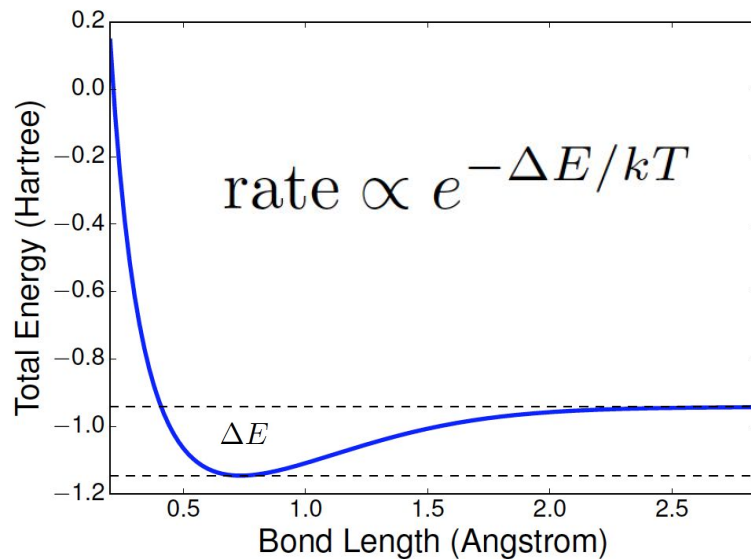
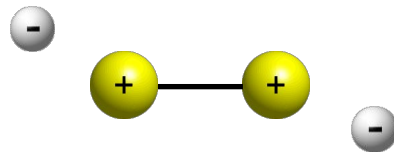
$$V_{pqrs} = \int dr_1 dr_2 \varphi_p^*(r_1) \varphi_q^*(r_2) \frac{1}{|r_1 - r_2|} \varphi_r(r_2) \varphi_s(r_1)$$

**Energy surfaces allow us to understand reactions**

Need chemical accuracy (1 kcal/mol) for rates

**Such accuracy is often classically intractable**

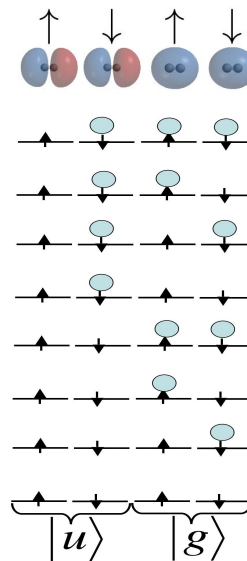
Especially for systems with strong correlation





# Representing $\eta$ electrons in $N$ spin-orbitals

## Second quantization requires $N$ qubits



$$\begin{aligned}
 H_{H_2} = & a_0 \mathbb{1} + a_1 (Z_0 + Z_1) + a_2 (Z_2 + Z_3) \\
 & + a_6 (Z_0 Z_3 + Z_1 Z_2) + a_7 (X_0 Y_1 Y_2 X_3 \\
 & + a_3 Z_0 Z_1 + a_4 Z_2 Z_3 + a_5 (Z_0 Z_2 + Z_1 Z_3) \\
 & + Y_0 X_1 X_2 Y_3 - X_0 X_1 Y_2 Y_3 - Y_0 Y_1 X_2 X_3)
 \end{aligned}$$

$$\begin{aligned}
 & \dots \\
 & \uparrow \downarrow \uparrow \downarrow \quad |0111\rangle \\
 & \uparrow \downarrow \uparrow \downarrow \quad |0110\rangle \\
 & \uparrow \downarrow \uparrow \downarrow \quad |0101\rangle \\
 & \uparrow \downarrow \uparrow \downarrow \quad |0100\rangle \\
 & \uparrow \downarrow \uparrow \downarrow \quad |0011\rangle \\
 & \uparrow \downarrow \uparrow \downarrow \quad |0010\rangle \\
 & \uparrow \downarrow \uparrow \downarrow \quad |0001\rangle \\
 & \uparrow \downarrow \uparrow \downarrow \quad |0000\rangle
 \end{aligned}$$

$$\{a_p, a_q^\dagger\} = a_p a_q^\dagger + a_q^\dagger a_p = \delta_{pq} \mathbb{1}$$

$$\{a_p, a_q\} = \{a_p^\dagger, a_q^\dagger\} = 0$$

$$\underbrace{\uparrow \downarrow}_{|u\rangle} \underbrace{\uparrow \downarrow}_{|g\rangle}$$

- Anti-symmetry is “encoded in the operators”
- Good near half filling or with compact basis

## First quantization requires $\eta \log N$ qubits

$\eta$  registers of size  $\log N$  index  
which orbital the particle occupies

$$\sum_{\phi_p \in \{\phi\}} a_{\phi_1 \dots \phi_\eta} |\phi_1 \dots \phi_i \dots \phi_j \dots \phi_\eta\rangle$$

$$= (-1)^\pi \sum_{\phi_p \in \{\phi\}} a_{\phi_1 \dots \phi_\eta} |\phi_1 \dots \phi_j \dots \phi_i \dots \phi_\eta\rangle$$

- Anti-symmetry is “explicit in the state”
- Ideal for high precision calculations

# Error-corrected quantum chemistry simulation

Science 309:5741 (2005), 1704-1707

1. Prepare an ansatz wavefunction  $\psi$  with “reasonable” support on the ground state

$$H |k\rangle = E_k |k\rangle \quad |\langle \psi | 0 \rangle|^2 = \text{not-too-small}$$

2. Form quantum circuit  $\mathbf{U} = \mathbf{e}^{-i f(H)}$  that encodes Hamiltonian spectrum in its eigenvalues

e.g., for Trotter:

$$f(H) = H = \sum_{\ell} H_{\ell} \quad U \approx \left( \prod_{\ell} e^{-i H_{\ell} / r} \right)^r$$

3. Application of  $\mathbf{U}$  to  $\psi$  accumulates phases  $f(E)$  encoding the spectrum

$$U |\psi\rangle = \sum_k \underbrace{\langle k | \psi \rangle}_{a_k} e^{-i f(E_k)} |k\rangle$$

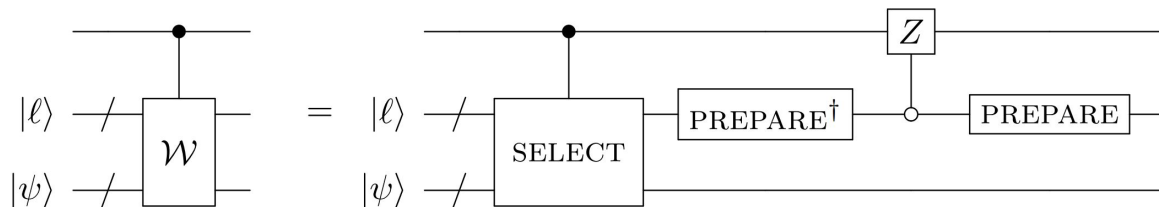
4. Phase estimation gives  $E_0$  with error  $\epsilon$  and probability  $|a_0|^2$  using  $\frac{1}{\epsilon} \left\| \frac{\partial f(E)}{\partial E} \right\|^{-1}$  queries to  $\mathbf{U}$



# Linear combination of unitaries (LCU) simulation

H as an “LCU”:  $H = \sum_{\ell=0}^{L-1} w_{\ell} U_{\ell}$  with 1-norm  $\lambda = \sum_{\ell=0}^{L-1} |w_{\ell}|$

“qubitization” (arXiv:1610.06546) synthesizes a quantum walk unitary:  $\mathcal{W} = e^{-i \arccos(H/\lambda)}$



$$\text{PREPARE } |0\rangle^{\otimes \log L} \mapsto \sum_{\ell=0}^{L-1} \sqrt{\frac{w_{\ell}}{\lambda}} |\ell\rangle$$

$$\text{SELECT } |\ell\rangle |\psi\rangle \mapsto |\ell\rangle U_{\ell} |\psi\rangle$$

Repeat this circuit  $\mathcal{O}(\lambda/\epsilon)$  times to estimate phase to within error  $\epsilon$

# But how does the quantum walk scale?

SELECT can be implemented at  $O(\eta)$  cost in first quantization,  $O(N)$  cost in second quantization

## PREPARE is the hard part

- Cost proportional to computation required to compute (or “load”) Hamiltonian coefficients

### Coulomb operator

$$\sum_{p,q,r,s=1} V_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

total cost =  $O(N^4 / \epsilon)$   
(1902.02134)

### Cholesky factorization

$$\sum_{\ell=1}^L \left( \sum_{\sigma \in \{\uparrow, \downarrow\}} \sum_{p,q=1}^{N/2} W_{pq}^{(\ell)} a_{p,\sigma}^\dagger a_{q,\sigma} \right)^2$$

total cost =  $O(N^{7/2} / \epsilon)$   
(1902.02134)

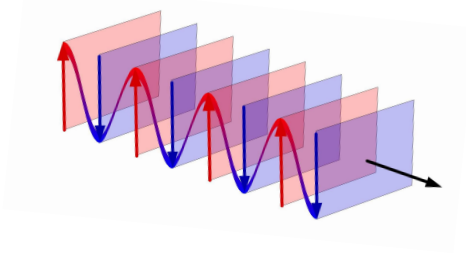
### Tensor hypercontraction

$$V_{pqrs} = \sum_{\mu, \nu=1}^{O(N)} \chi_p^{(\mu)} \chi_q^{(\mu)} \zeta_{\mu\nu} \chi_r^{(\nu)} \chi_s^{(\nu)}$$

total cost =  $O(N^3 / \epsilon)$   
(2011.03494)

# First quantization and simple basis sets

Simple basis sets like grids, plane waves lead to analytic integrals!



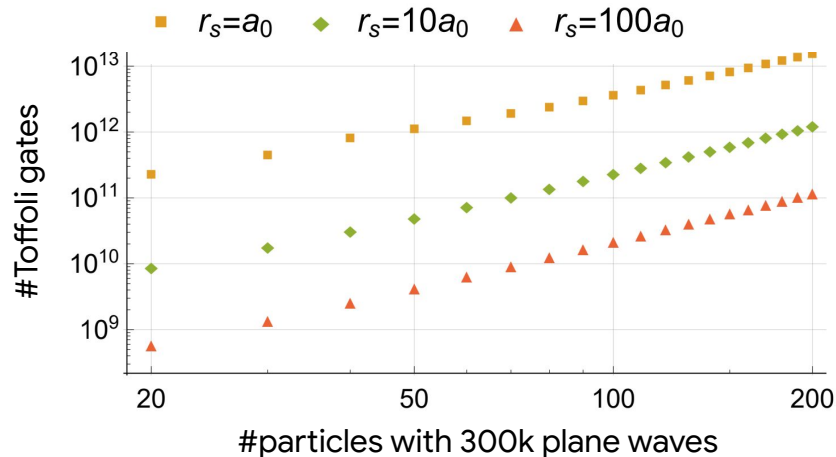
$$V = \frac{2\pi}{\Omega} \sum_{\substack{p \neq q \\ \nu \neq 0}} \frac{c_{p+\nu}^\dagger c_{q-\nu}^\dagger c_q c_p}{k_\nu^2}$$

But molecules need 100X - 1,000X more plane waves than MOs to reach chemical accuracy

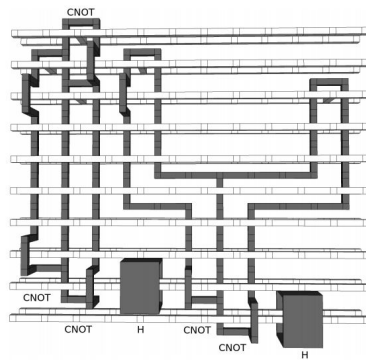
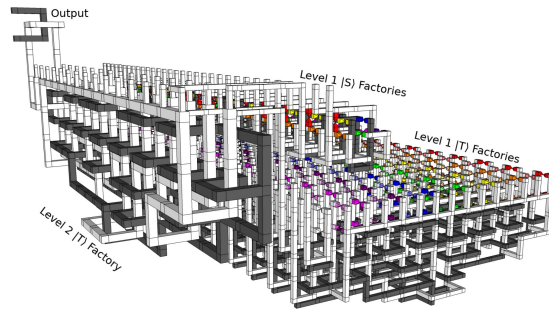
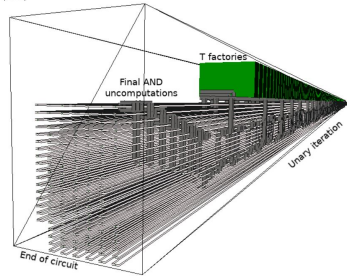
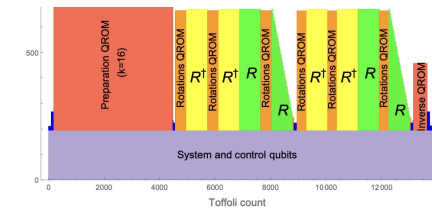
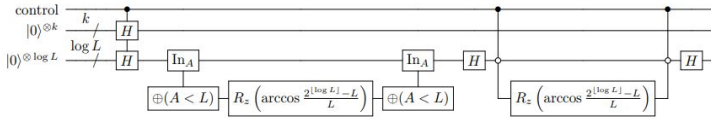
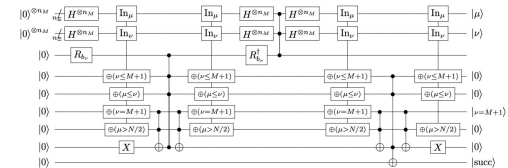
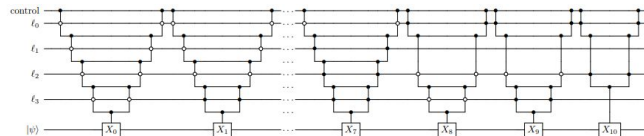
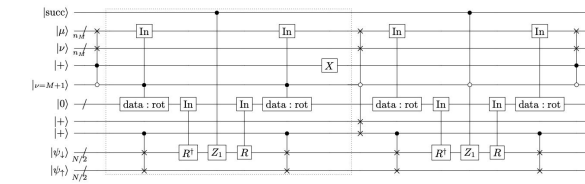
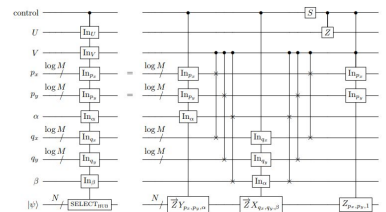
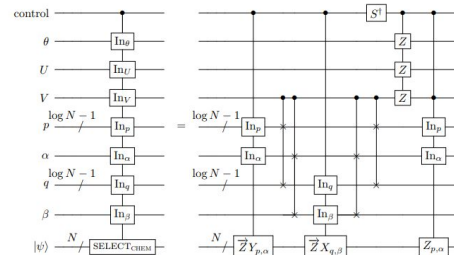
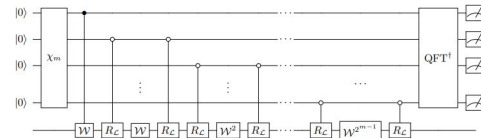
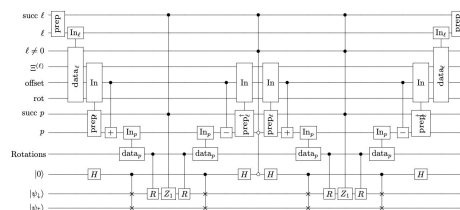
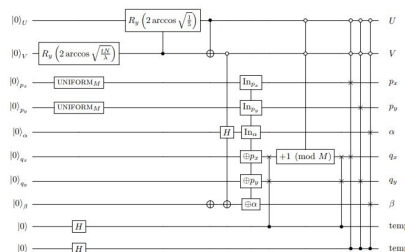
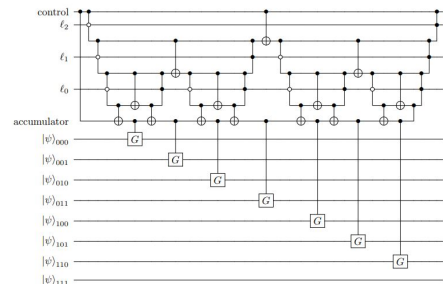
- In second quantization, space complexity is  $O(N)$
- Would need 100k logical qubits instead of 100!

In first quantization, space complexity is  $O(\eta \log N)$

- 60 electrons in 100k PWs needs ~1k logical qubits
- $1807.09802 + 2105.12767$  scale as low as  $O(\eta^{8/3} N^{1/3})$
- Particularly attractive for non-BO dynamics



# Compilation is tedious, often thankless work



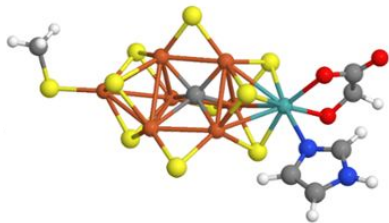
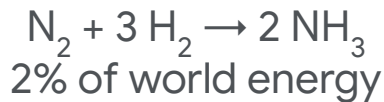


## Part III: searching for applications of these algorithms





# FeMoCo is great but we need more



| Year | arXiv                      | Method                                    | Space                          | T Complexity                                 | T Gates        | Physical qubits    |
|------|----------------------------|---|--------------------------------|--|----------------|--------------------|
| 2005 | <a href="#">0604193</a>    | Trotter                                   | $\mathcal{O}(N)$               | $\mathcal{O}(\text{poly}(N/\epsilon))$       | Unknown        | Unknown            |
| 2010 | <a href="#">1001.3855</a>  | Trotter (first bounds on step complexity) | $\mathcal{O}(N)$               | $\tilde{\mathcal{O}}(N^{11}/\epsilon^{3/2})$ | Unknown        | Unknown            |
| 2013 | <a href="#">1312.1695</a>  | Trotter (first bounds on number of steps) | $\mathcal{O}(N)$               | $\tilde{\mathcal{O}}(N^9/\epsilon^{3/2})$    | Unknown        | Unknown            |
| 2014 | <a href="#">1406.4920</a>  | Trotter (tighter bounds)                  | $\mathcal{O}(N)$               | $\tilde{\mathcal{O}}(N^6/\epsilon^{3/2})$    | Unknown        | Unknown            |
| 2015 | <a href="#">1506.01020</a> | Taylor series                             | $\mathcal{O}(N)$               | $\tilde{\mathcal{O}}(N^5/\epsilon)$          | Unknown        | Unknown            |
| 2016 | <a href="#">1605.03590</a> | Trotter (first resource estimate)         | $\mathcal{O}(N)$               | $\tilde{\mathcal{O}}(N^6/\epsilon^{3/2})$    | $\sim 10^{14}$ | $\sim 20\text{MM}$ |
| 2019 | <a href="#">1902.02134</a> | qubitization + single factorization       | $\tilde{\mathcal{O}}(N^{3/2})$ | $\tilde{\mathcal{O}}(N^4/\epsilon)$          | $\sim 10^{11}$ | $\sim 6\text{MM}$  |
| 2020 | <a href="#">2007.14460</a> | qubitization + double factorization       | $\tilde{\mathcal{O}}(N^{3/2})$ | $\tilde{\mathcal{O}}(N^{7/2}/\epsilon)$      | $\sim 10^{10}$ | $\sim 4\text{MM}$  |
| 2020 | <a href="#">2011.03494</a> | qubitization + tensor hypercontraction    | $\tilde{\mathcal{O}}(N)$       | $\tilde{\mathcal{O}}(N^3/\epsilon)$          | $\sim 10^9$    | $\sim 2\text{MM}$  |

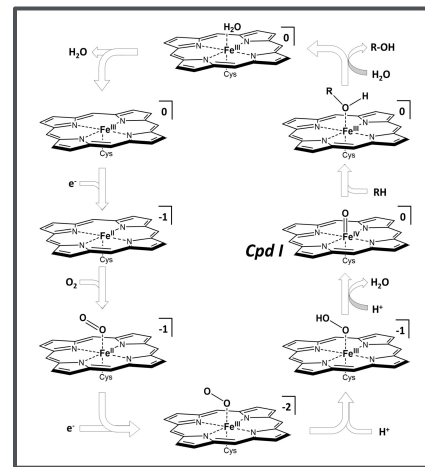
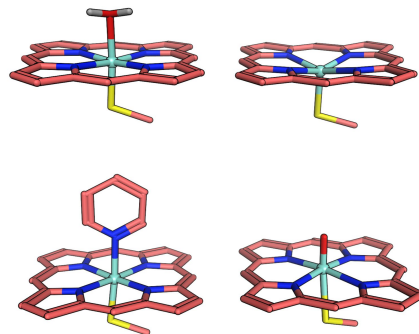
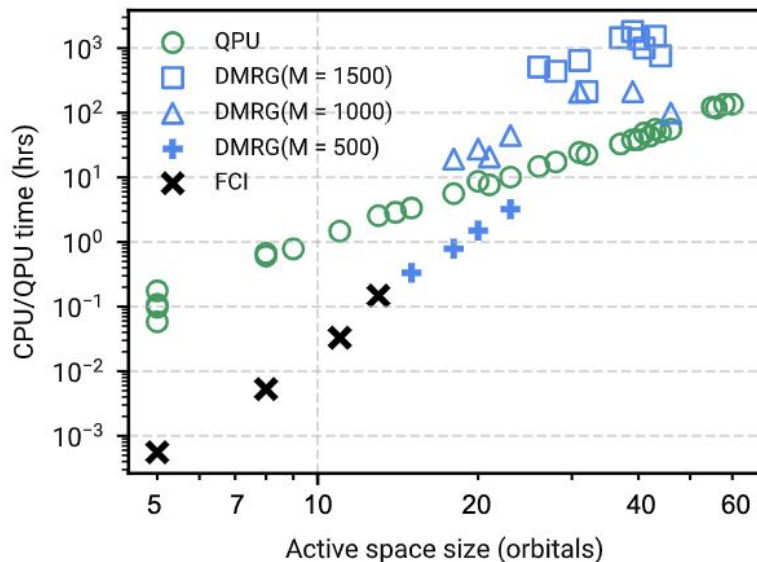
TABLE I. Best fault-tolerant algorithms for phase estimating chemistry in an arbitrary (e.g., molecular orbital) basis.  $N$  is number of basis functions and  $\epsilon$  is target precision. Gate counts are for FeMoCo, physical qubit counts assume superconducting qubit surface code implementation (see most recent papers for further assumptions).

- Critical to flesh out more specifically what valuable technological problems might be practically solved with a few thousand logical qubits and  $< 10^{12}$  Toffoli gates

# Assessing quantum/classical boundary for P450

PNAS 119, 2203533119 (2022)

P450 is strongly correlated  
iron-porphyrin / drug anti-target  
(kind of like FeMoCo!)

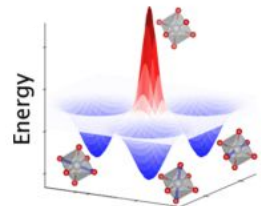


We observe onset of quantum advantage for  
active space sizes near 80 qubits

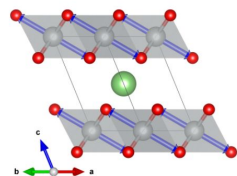
Chemically relevant (and classically intractable)  
calculations would require ~3k qubits,  $\sim 10^{10}$  Toffolis

# Ab initio materials simulation is still very costly

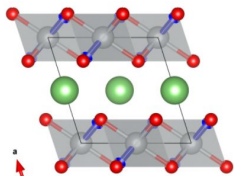
PRX Quantum 4, 040303 (2023)



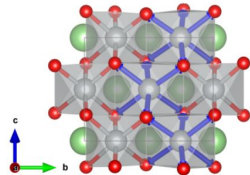
Want to get Co out of batteries, LNO is good candidate, why not Jahn-Teller distorted?



$C2/m$   
(collinear Jahn-Teller)



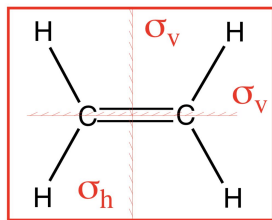
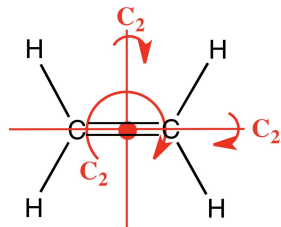
$P2_1/c$   
(zig-zag Jahn-Teller)



$P2/c$   
(disproportionated)

- Classical many-body methods unreliable for metals
- Embedding difficult to converge finite size
- DFT disagrees between functionals

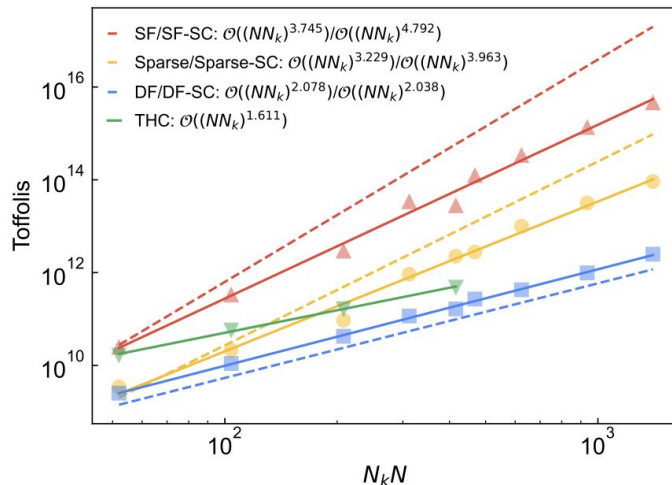
recent work symmetry adapts qubitization



| $\Gamma_{ij}$ | $a'$ | $a'$ | $a'$ | $a'$ | $a'$ | $a''$ | $a''$ | $a''$ | $a''$ |
|---------------|------|------|------|------|------|-------|-------|-------|-------|
| $i$           | 0    | 0    | 1    | 1    | 2    | 0     | 1     | 2     | 2     |
| $j$           | 0    | 1    | 0    | 1    | 2    | 2     | 0     | 1     | 2     |

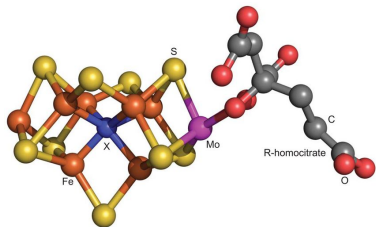
| $\Gamma_{ij}$ | $k$ | $b$ |
|---------------|-----|-----|
| $a'$          | 0   | 0   |
| $a'$          | 0   | 1   |
| $a'$          | 1   | 0   |
| $a'$          | 1   | 1   |
| $a'$          | 2   | 2   |
| $a'$          | 2   | 3   |
| $a''$         | 0   | 2   |
| $a''$         | 0   | 3   |
| $a''$         | 1   | 2   |
| $a''$         | 1   | 3   |
| $a''$         | 2   | 0   |
| $a''$         | 2   | 1   |

  
 $A_1 \subset \Gamma_p \otimes \Gamma_q \otimes \Gamma_r \otimes \Gamma_s$ 


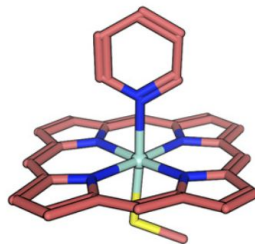
Gives linearly reduced scaling in number of k-points

**Q algorithms must further improve for viability**

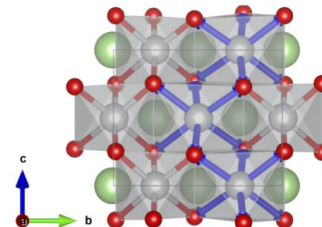
# Are only the most highly entangled systems promising applications of quantum simulation?



FeMoCo (fertilizer catalyst)  
PRX Quantum 2, 030305 (2021)



P450 (drug anti-target)  
PNAS 119, 2203533119 (2022)



LiNiO<sub>2</sub> (battery cathode)  
PRX Quantum 4, 040303 (2023)

- “classical competition” is only the most costly/accurate methods (e.g. AFQMC, DMRG)

**most chemical computations do *not* require accurate treatment of strong correlation**

- “classical competition” is highly efficient/approximate classical methods (e.g. mean-field, DFT)
- super-quadratic quantum advantage over mean-field would **dramatically** broaden applications

# Super-quadratic quantum advantage over classical mean-field methods possible for electron dynamics

Nat. Comm 14, 4058 (2023)

## Usual quantum sim. advantage is resolution of entanglement

- storing wavefunction with  $\eta$  particles,  $N$  orbitals classically requires  $O(N \text{ choose } \eta)$  bits
- mean-field has no particle correlation, only requires  $O(N \eta)$  bits and gate complexity:

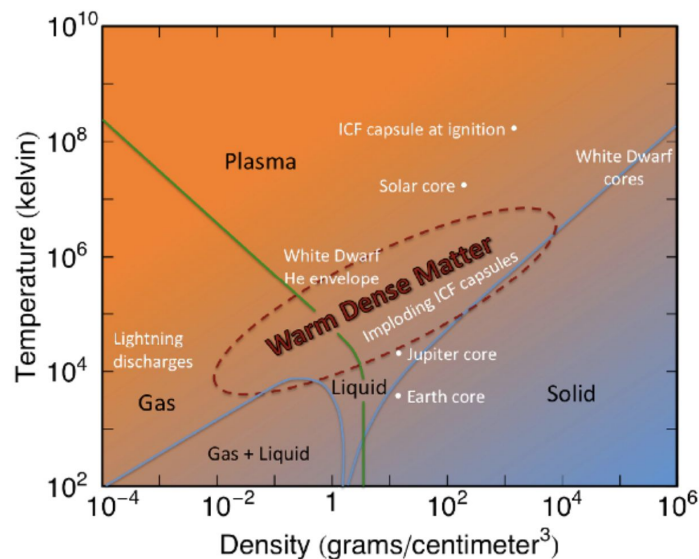
$$N^{4/3} \eta^{7/3} t + N^{5/3} \eta^{4/3} t$$

or, for high temperature:

$$N^{10/3} \eta^{1/3} t + N^{11/3} t / \eta^{2/3}$$

quantum simulations need only  $O(\eta \log N)$  qubits and gate complexity:

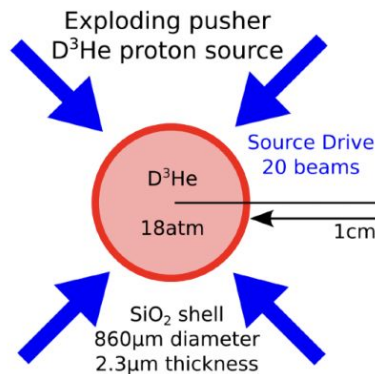
$$N^{1/3} \eta^{8/3} t$$



# Quantum simulating heating of pre-ignition ICF

**“The essence of controlled laboratory thermonuclear fusion is to use the fusion product’s kinetic energy to self-heat the plasma, accelerating and perpetuating the burn”**

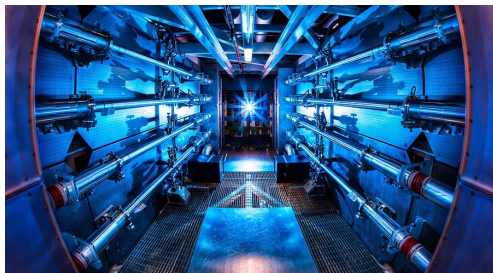
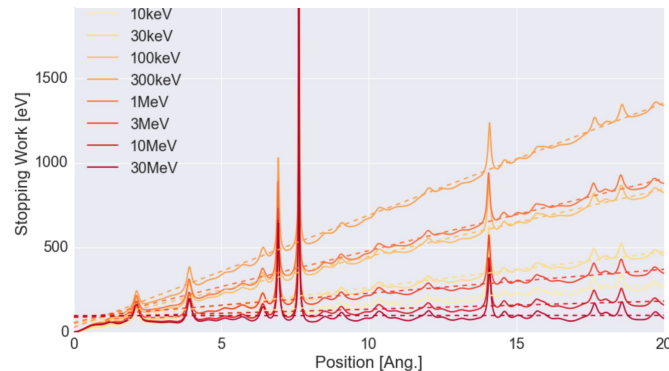
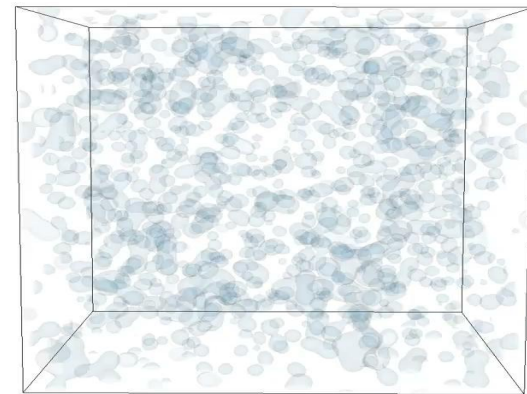
*Phys. Plasmas 26, 062701 (2019)*



Stopping power = rate at which a material absorbs kinetic energy of charged particle passing through it

Multiscale ICF modeling depends sensitively on “stopping power” as a function of temperature, velocity

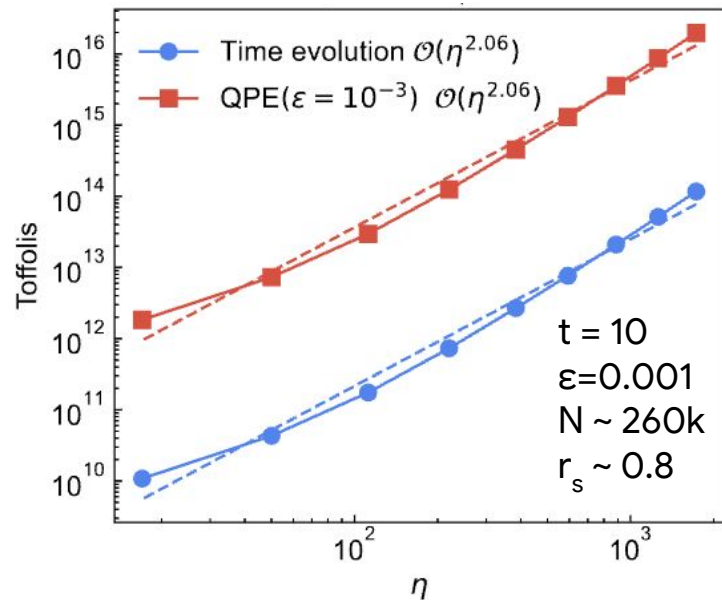
DOE spends billions of CPU hours per year running inaccurate TDDFT for stopping power





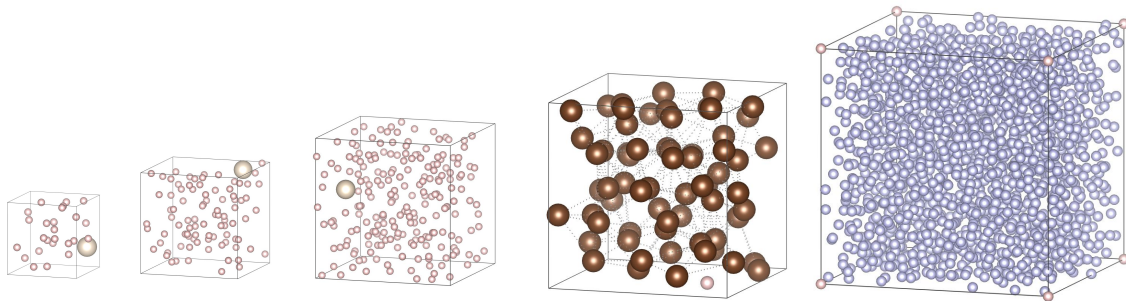
# Resource estimates for stopping power

arXiv:2308.12352



*reference benchmarks*

- **FeMoCO**: 2100 Qubits,  $3.2 \times 10^{10}$  Toffoli
- **P450**: 1500 Qubits,  $7.0 \times 10^9$  Toffoli



| Projectile + Host       | $\eta$ | QSP Toffoli            | Trotter Toffoli        | QSP Qubits | Trotter Qubits |
|-------------------------|--------|------------------------|------------------------|------------|----------------|
| Helium + Hydrogen (50%) | 28     | $1.166 \times 10^{14}$ | $2.143 \times 10^{12}$ | 1749       | 444            |
| Helium + Hydrogen (75%) | 92     | $4.239 \times 10^{15}$ | $5.852 \times 10^{13}$ | 3309       | 1680           |
| Helium + Hydrogen       | 218    | $4.154 \times 10^{16}$ | $2.667 \times 10^{14}$ | 5650       | 3948           |
| Hydrogen+Deuterium      | 1729   | $4.424 \times 10^{19}$ | $3.964 \times 10^{16}$ | 33038      | 31146          |
| Hydrogen + Carbon       | 391    | $4.640 \times 10^{17}$ | $2.049 \times 10^{15}$ | 8841       | 7062           |



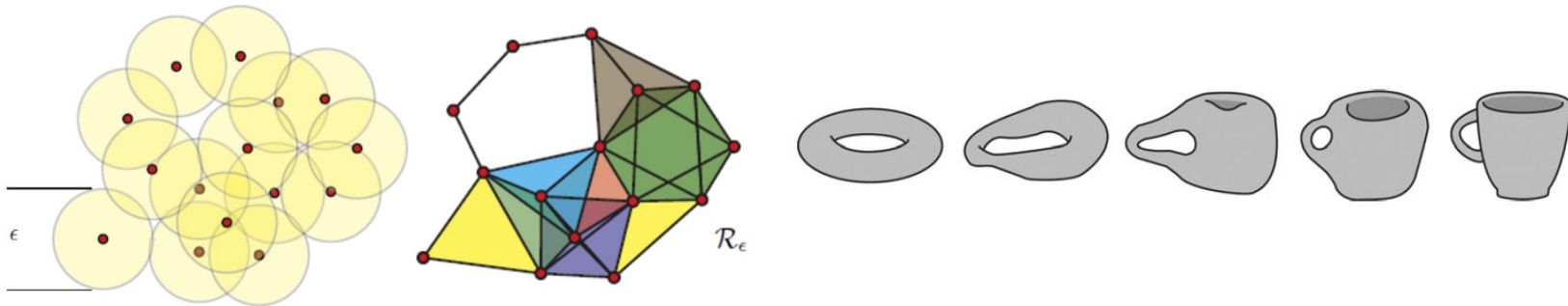


## Part IV: case study on the viability of quantum topological data analysis



# What is topological data analysis?

- Given  $n$  data points, make a graph  $G$  with data points as nodes, with edges between points wherever the points are within some distance (“filtration”)  $\epsilon$



- The  $k^{\text{th}}$  order Betti number ( $\beta_k$ ) is the number of  $k$ -dimensional holes in the simplicial complex
- Topological features are somewhat fundamental global properties, often robust to noise in data
- Real world applications of this in neuroscience, epidemiology, genetics, finance, even physics



# Quantum algorithms for topological and geometric analysis of data

Seth Lloyd<sup>1</sup>, Silvano Garnerone<sup>2</sup> & Paolo Zanardi<sup>3</sup>

Extracting useful information from large data sets can be a daunting task. Topological methods for analysing data sets provide a powerful technique for extracting such information. Persistent homology is a sophisticated tool for identifying topological features and for determining how such features persist as the data is viewed at different scales. Here we present quantum machine learning algorithms for calculating Betti numbers—the numbers of connected components, holes and voids—in persistent homology, and for finding eigenvectors and eigenvalues of the combinatorial Laplacian. The algorithms provide an exponential speed-up over the best currently known classical algorithms for topological data analysis.

# The quantum approach to TDA

Nat. Comms. 7: 10138 (2016)

- Every data point (node) is represented by a qubit, with every computational basis state representing a clique; e.g.,  $|01101\rangle$  is a clique between nodes 2,3,5
1. Prepare the equal mixed state over  $Cl_k(G)$ , all  $k$ -cliques in the simplicial complex  
→ can be accomplished via amplitude amplification from Dicke state of order  $k$
  2. Apply phase estimation to the combinatorial Laplacian associated with the data graph  $G$
  3. Estimate  $\beta_k$  as the dimension of the kernel of that combinatorial Laplacian
- The most natural thing to estimate from this procedure is actually an approximate Betti number normalized by the number of  $k$ -cliques, i.e.  $\beta_k / |Cl_k(G)|$



# Algorithm improvements from our work

see [arXiv:2209.13581](https://arxiv.org/abs/2209.13581)

- New method based on threshold testing to prepare a mixture of fixed Hamming-weight states with garbage information that has significantly lower fault-tolerant cost
- Directly perform phase estimation on the quantum walk operator
- Use Kaiser windows functions to reduce the number of amplitude estimation steps
- Project onto the kernel of the boundary map by implementing a Chebyshev polynomial to optimally filter zero eigenvalues from phase estimation
- Use overlap estimation to estimate kernel dimension of block-encoded combinatorial Laplacian, leading to a quadratic improvement in precision over prior work



# Quantum resource analysis

see [arXiv:2209.13581](https://arxiv.org/abs/2209.13581)

**Classical cost:  $O(\binom{n}{k})$**

$n$  = number of nodes/qubits

$|E|$  = number of edges

$\beta_k^G$  =  $k^{\text{th}}$  order Betti number of graph  $G$

$\delta$  = success probability

**Cost in terms of  $\alpha$ , the additive error in  $\beta_k^G$ :**

$$6|E| \frac{\ln(1/\delta)}{\alpha} \sqrt{|\text{Cl}_k(G)| \beta_{k-1}^G} \left[ \frac{\pi}{2} \sqrt{\frac{\binom{n}{k}}{|\text{Cl}_k(G)|}} + \frac{n}{\lambda_{\min}} \ln \left( \frac{4|\text{Cl}_k(G)|}{\alpha} \right) \right]$$

**Cost in terms of  $r$ , the multiplicative (e.g. percent) error in  $\beta_k^G$ :**

$$6|E| \frac{\ln(1/\delta)}{r} \sqrt{\frac{|\text{Cl}_k(G)|}{\beta_{k-1}^G}} \left[ \frac{\pi}{2} \sqrt{\frac{\binom{n}{k}}{|\text{Cl}_k(G)|}} + \frac{n}{\lambda_{\min}} \ln \left( \frac{4|\text{Cl}_k(G)|}{r \beta_{k-1}^G} \right) \right]$$

# Quantum resource analysis

see [arXiv:2209.13581](https://arxiv.org/abs/2209.13581)

**Classical cost:  $O(\binom{n}{k})$**

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**Cost in terms of  $\alpha$ , the additive error in  $\beta_k^G$ :**

$$3\pi|E|\frac{\ln(1/\delta)}{\alpha}\sqrt{\binom{n}{k}\beta_{k-1}^G}$$

- Never more than quadratic quantum speedup
- Implies practical advantage is unlikely

**Cost in terms of  $r$ , the multiplicative (e.g. percent) error in  $\beta_k^G$ :**

$$3\pi|E|\frac{\ln(1/\delta)}{r}\sqrt{\frac{\binom{n}{k}}{\beta_{k-1}^G}}$$

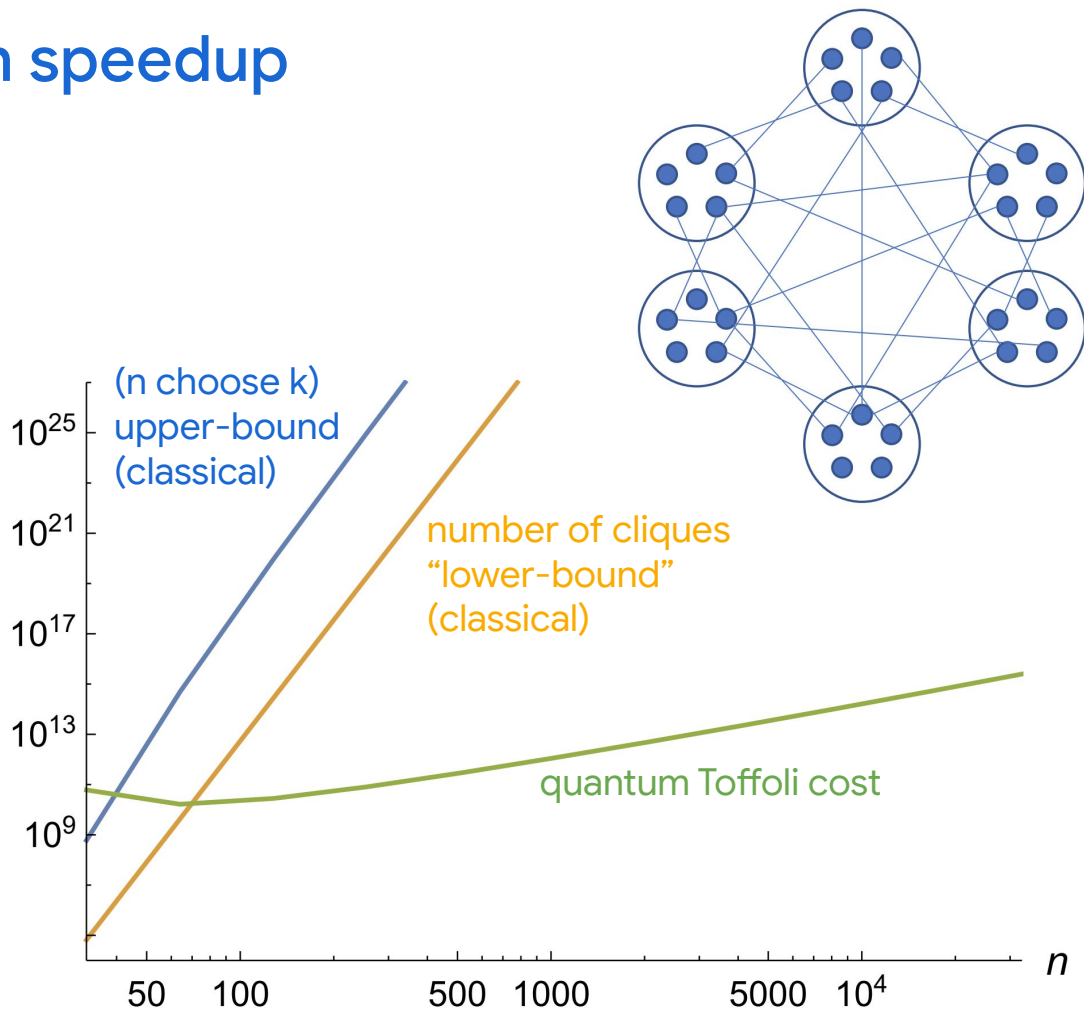
- Quantum speedup only when  $\beta_k^G$  is large
- Exponential iff  $\beta_k^G = \Omega(\binom{n}{k} / \text{poly}(n, k))$



# Problem instances with speedup

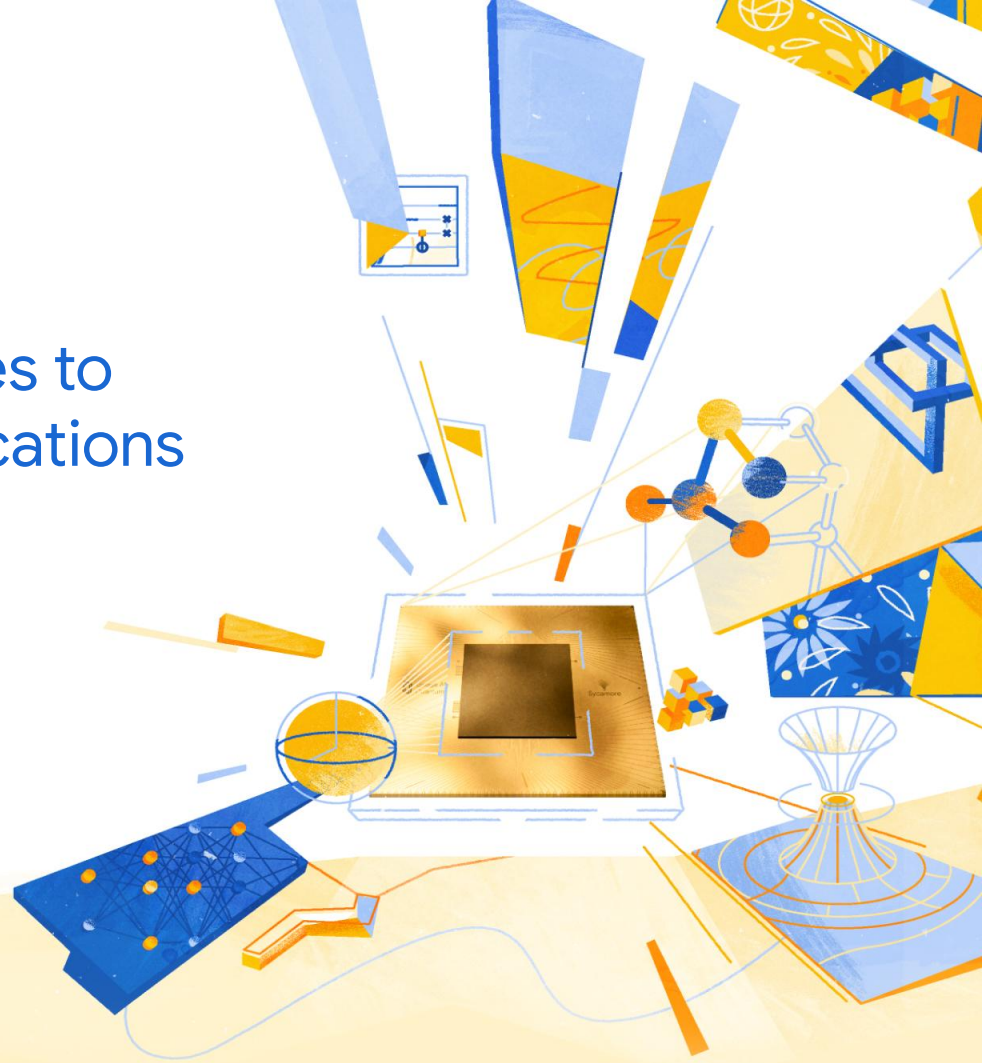
see [arXiv:2209.13581](https://arxiv.org/abs/2209.13581)

- We construct graphs with Betti number large enough for superpolynomial speedup
- Do real applications have speedup?
- Erdos-Renyi graphs with edge with probability  $p$  have mean Betti number  $(n \text{ choose } k+1) / p^{(k+1 \text{ choose } 2)}$
- Optimal  $p$  gives quartic speedup





## Part III: other interesting places to look for viable quantum applications



# Exponential speedup in simulating classical oscillators

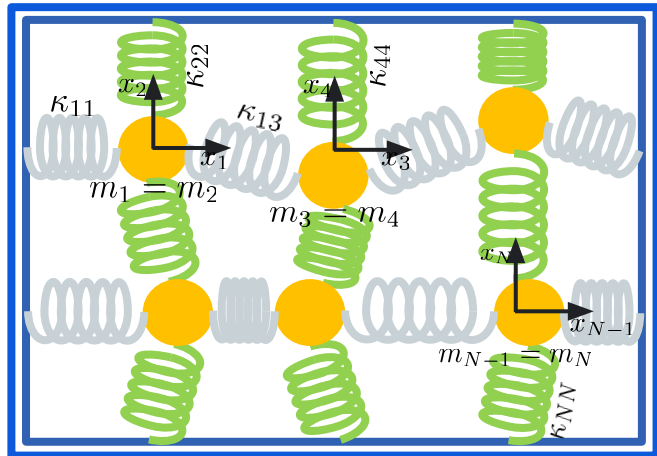
PRX 13, 041041 (2023) + FOCS 2023

Hooke's Law for coupled oscillators can be expressed as:

$$\ddot{\vec{y}}(t) = -A\vec{y}(t)$$

Adding  $i\sqrt{A}\dot{\vec{y}}(t)$  to both sides gives Schrodinger equation:

$$\frac{d}{dt} \left( \dot{\vec{y}}(t) + i\sqrt{A}\vec{y}(t) \right) = i\sqrt{A} \left( \dot{\vec{y}}(t) + i\sqrt{A}\vec{y}(t) \right)$$

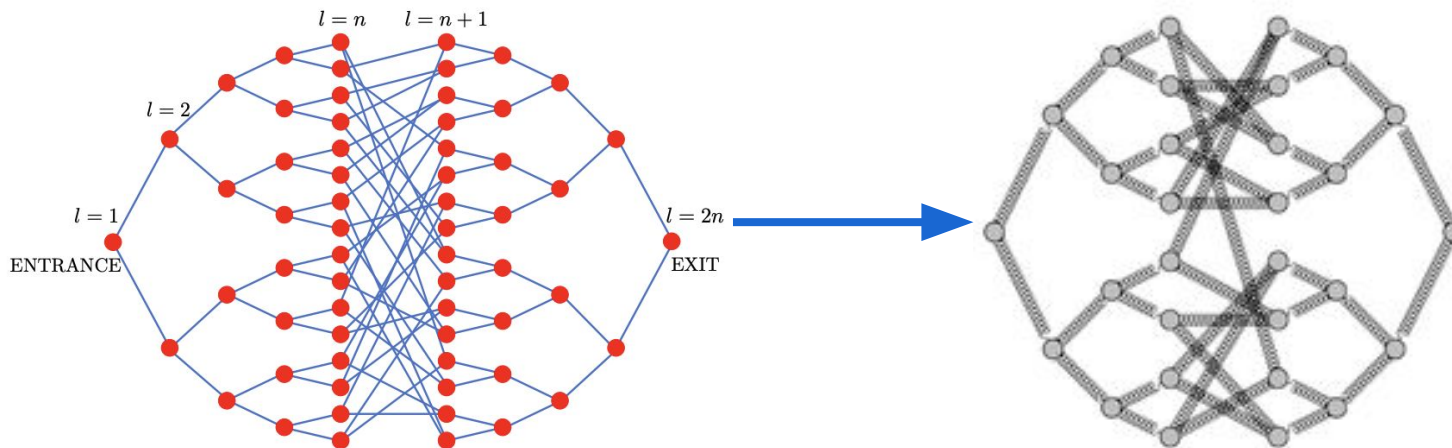


- If spring constants/masses efficiently computable, can simulate N oscillators in  $O(\text{polylog}(N))$
- Many potential applications: modeling electrical grids, mechanical engineering, classical wave equation, molecular vibrations, statistical mechanics of fields, etc.

# Exponential speedup in simulating classical oscillators

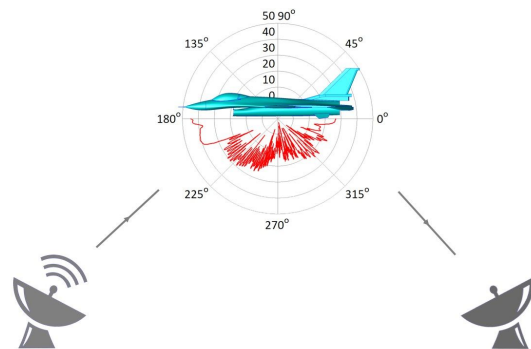
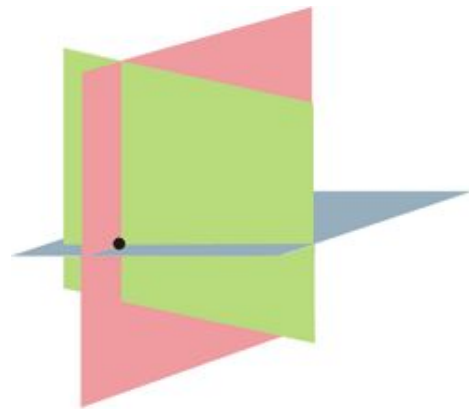
PRX 13, 041041 (2023) + FOCS 2023

- We prove that measuring kinetic energy of an oscillator is BQP-Complete  
Even when all masses are the same and there are two spring constants
- We also show relativized exponential speedup in an oracle model, leveraging glued trees



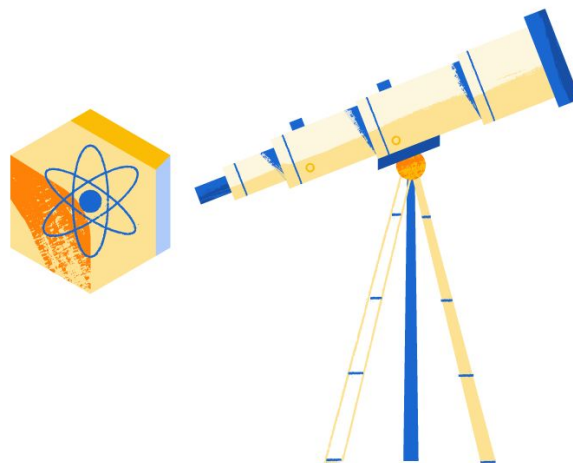
# Searching for applications of quantum linear algebra

- Quantum computers can solve systems of  $N$  linear equations ( $A \mathbf{x} = \mathbf{b}$ ) “querying”  $A$  only  $O(\text{polylog}(N))$  times 😊
- But sometimes each queries to  $A$  or  $\mathbf{b}$  take time  $O(\text{poly}(N))$  😞
- Focus on problems where linear system has underlying structure, e.g., physically inspired linear differential equations
- Should avoid situations where sampling the output is efficient via Monte Carlo (e.g. options pricing, Fokker-Planck, heat equation, etc.)
- Promising directions include acoustic or electromagnetic scattering, fluid dynamics with certain constraints, plasma physics, etc.





Classical Data



Quantum Data

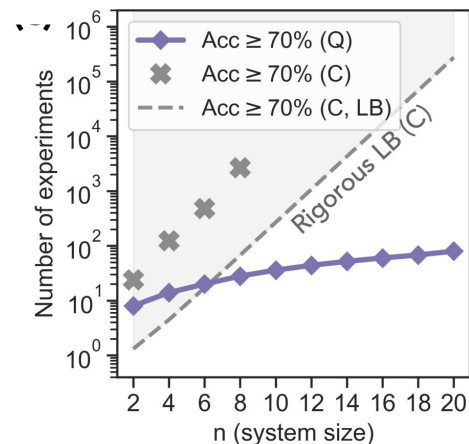
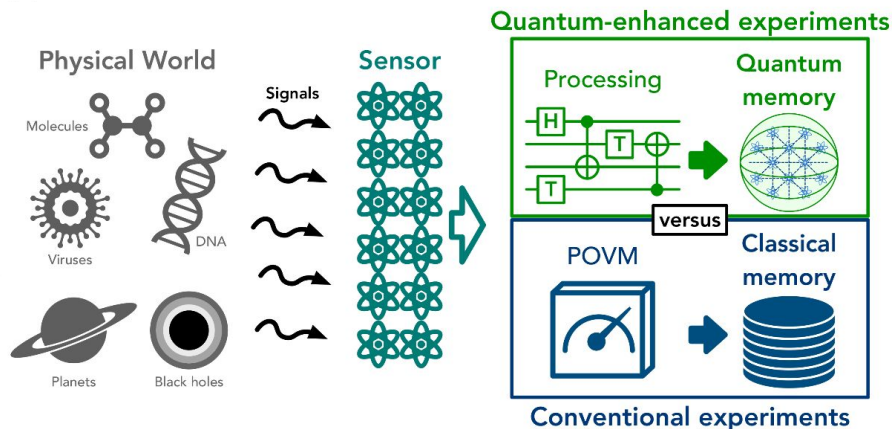
Whether starlight or molecular spectra, thus far science has only used “classical data”

If data is collected by quantum sensor (rapidly progressing technology) and transduced to an error-corrected quantum memory, we can do amazing things with that data

Quantum states output from a quantum simulation (e.g. of chemistry) also constitute quantum data

# Quantum enhanced experiments

Science 376, 1182–1186 (2022)



By entangling two copies of  $N$  qubit state (e.g. from a sensor), we can learn properties with  $2^N$  fewer queries vs single copy

With limited data, one can achieve quantum advantage with very few qubits



# How will a modest error-corrected quantum computer impact the world?

- We have a responsibility to answer this question with more clarity
- Simulations of molecules and materials remain promising
  - Molecular ground states in scope if strongly correlated
  - Many initio solid-state applications but resource requirements very high
  - Can outperform classical mean-field when goal is dynamics
- Computing stopping power of pre-ignition fusion fuels has decisive quantum advantage, corresponds to relevant real-world experiments for  $10^{12}$  –  $10^{13}$  Toffoli gates
- Interesting other applications include topological data analysis, simulating certain classical differential equations, analysis of data from quantum sensors or simulations





Quantum AI

Thank you!

Bill Huggins  
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Dominic Berry  
Edward Farhi  
Fionn Malone  
Joonho Lee  
Kianna Wan  
Marika Kieferova

Matthew Harrigan  
Mike Freedman  
Nicholas Rubin  
Ramis Movassagh  
Robert Huang  
Robin Kothari  
Rolando Somma  
Stephen Jordan  
Tanuj Khattar  
Thomas O'Brien

Google

