



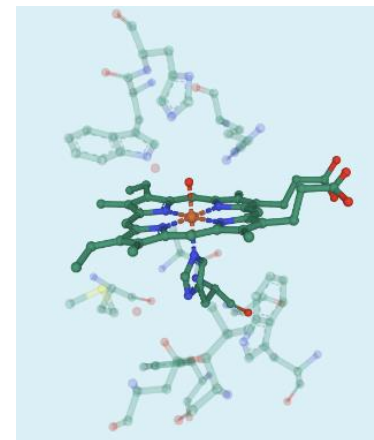
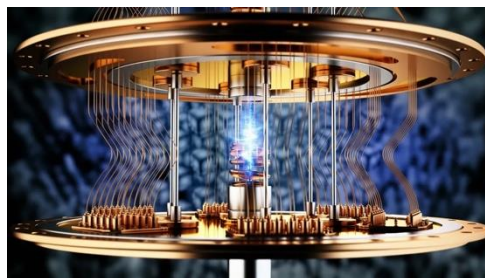
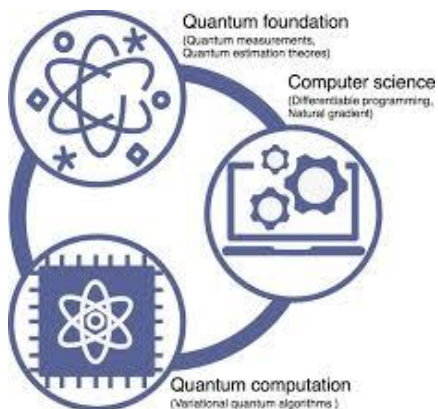
HCMUS

Viet Nam National University
Ho Chi Minh City
University of Science

Quantum computing for many-body simulation, optimization and machine learning

Tran Nguyen Lan

University of Science – VNUHCM



Aug 22

QuantumLab@HCMUS

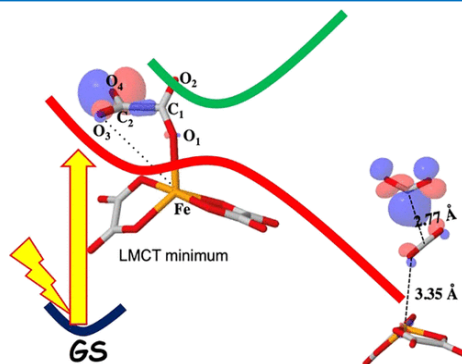
Electronic-structure methods

$$E = \langle 0 | e^{\hat{A}_{\text{int}}^\dagger} e^{\hat{A}_{\text{ext}}^\dagger} \hat{H} e^{\hat{A}_{\text{ext}}} e^{\hat{A}_{\text{int}}} | 0 \rangle$$

$$= \langle 0 | e^{\hat{A}_{\text{int}}^\dagger} \hat{H}_{\text{ext}} e^{\hat{A}_{\text{int}}} | 0 \rangle$$



Excited states and Dynamics



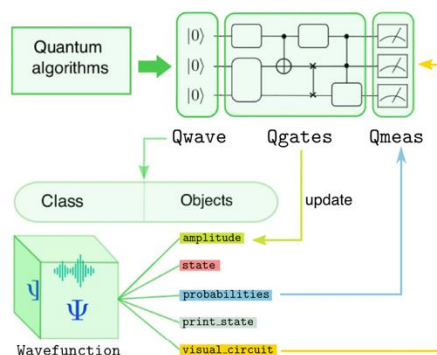
In collaboration with:

- Prof. Phan N. Loan, HCMUE
- Dr. Huynh T. Duc, VAST
- Dr. Le B. Ho, Tohoku, Japan
- Dr. Nguyen T. Hoang, VAST

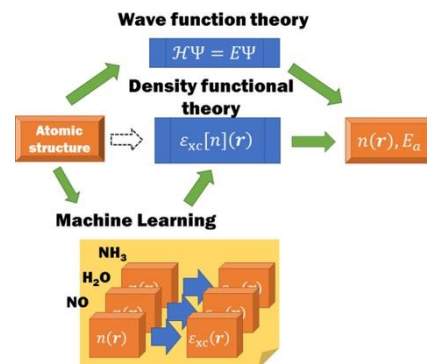
30 members



Quantum computing and information



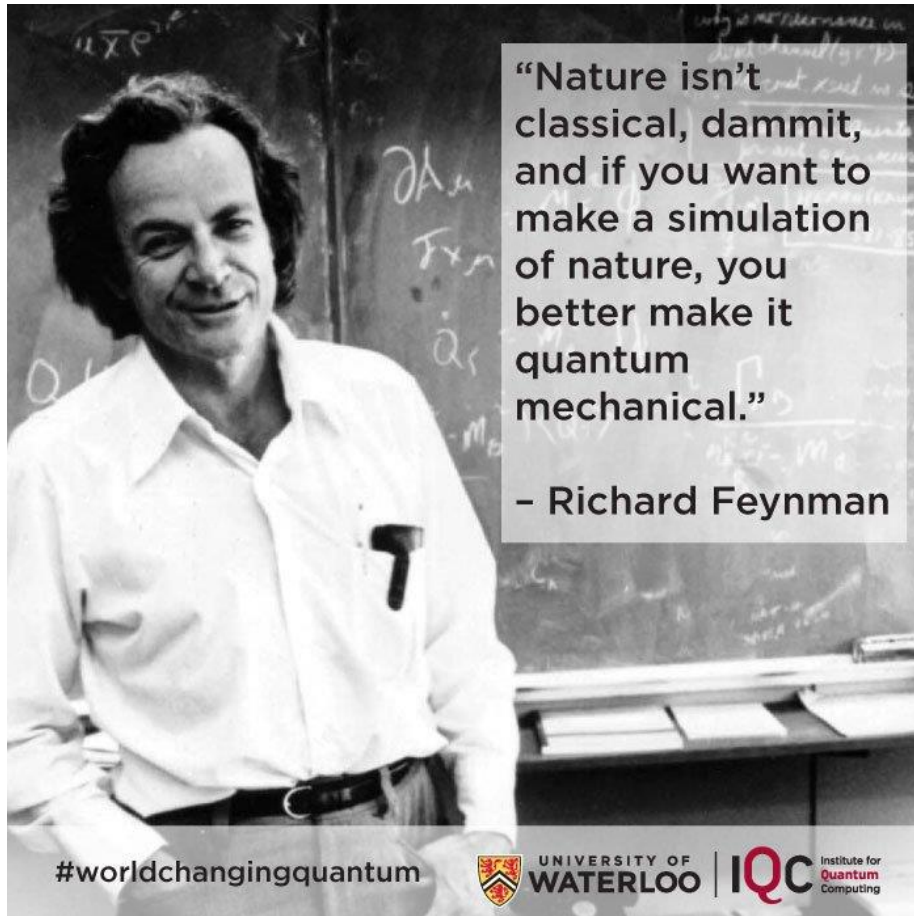
Machine learning for many-body physics



Outline

1. Intro to Quantum computing (QC)?
2. Quantum many-body simulation
3. Quantum optimization
4. Quantum machine learning
5. Summary

1. Intro to quantum computing?



“Nature isn’t classical, dammit, and if you want to make a simulation of nature, you better make it quantum mechanical.”

– Richard Feynman

#worldchangingquantum



UNIVERSITY OF
WATERLOO

IQC

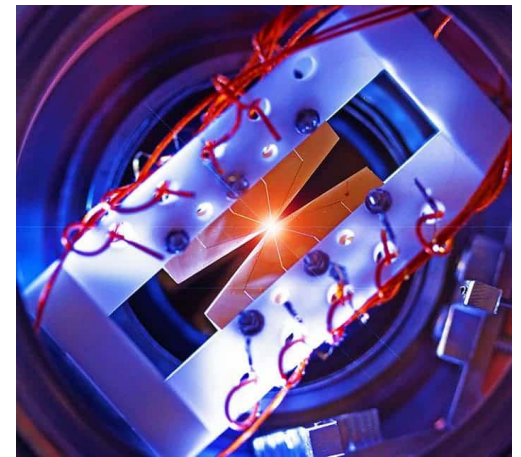
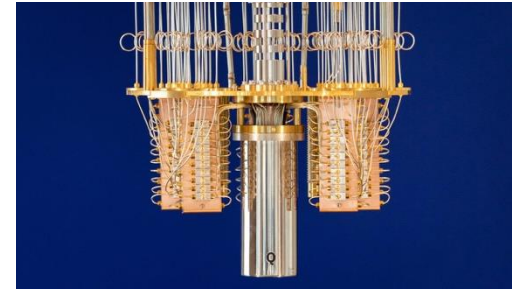
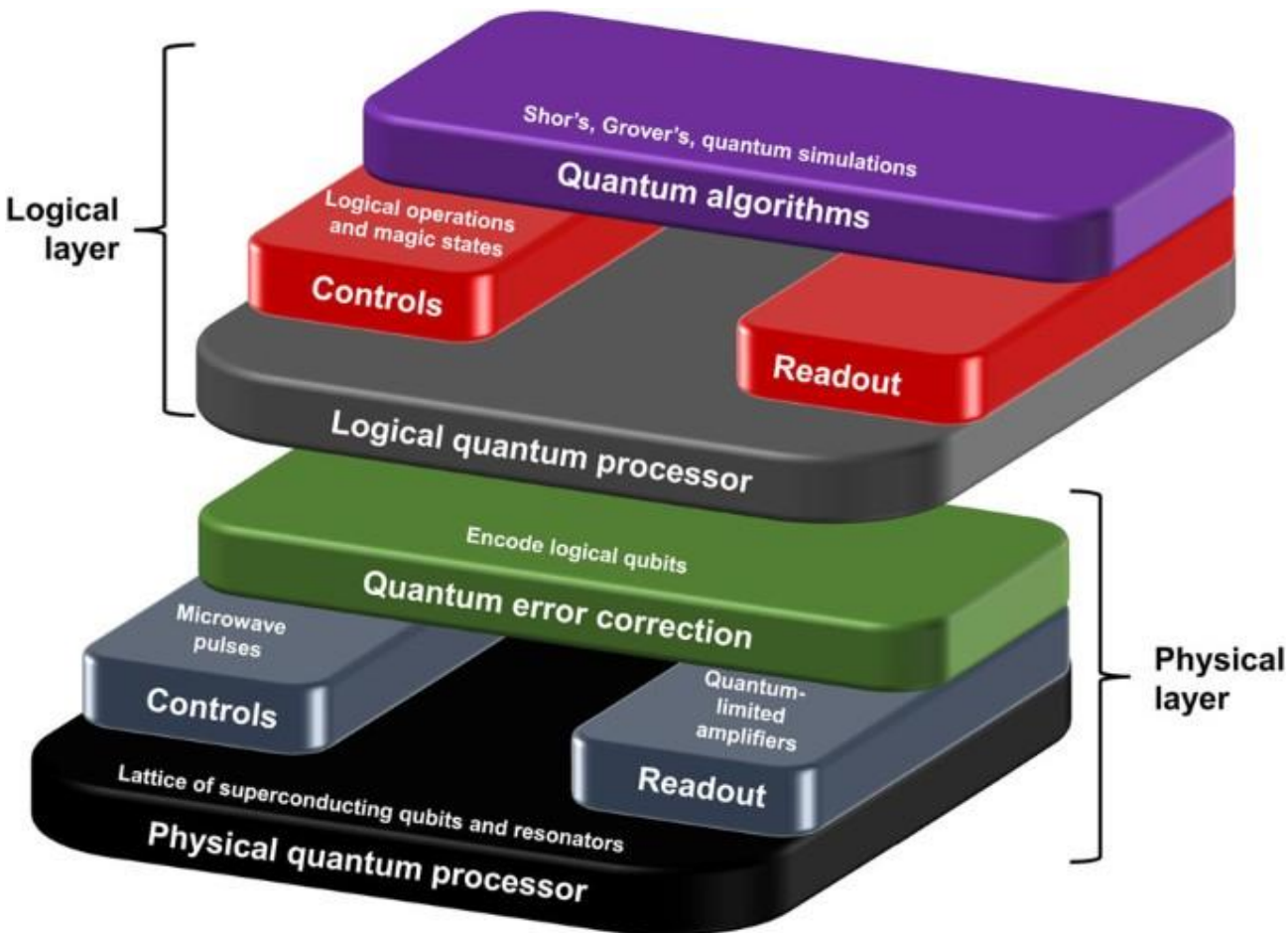
Institute for
Quantum
Computing

Quantum computing is a multidisciplinary field comprising aspects of computer science, physics, and mathematics **that utilizes quantum mechanics to solve complex problems faster than on classical computers.**



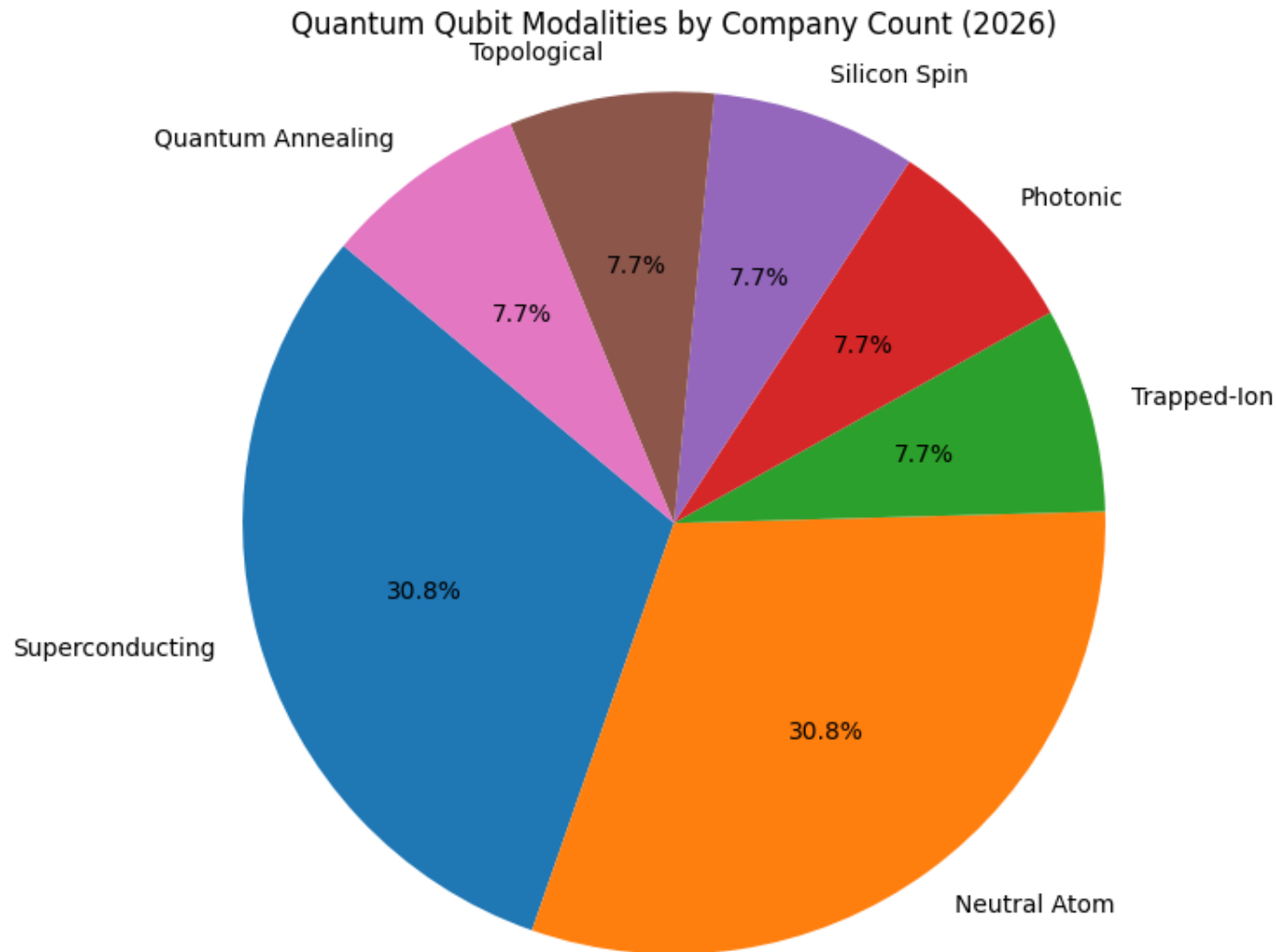
“Quantum Willow chip, 105 qubits, is **10^{25} times faster than** supercomputer.” [2025]

1. Intro to quantum computing?



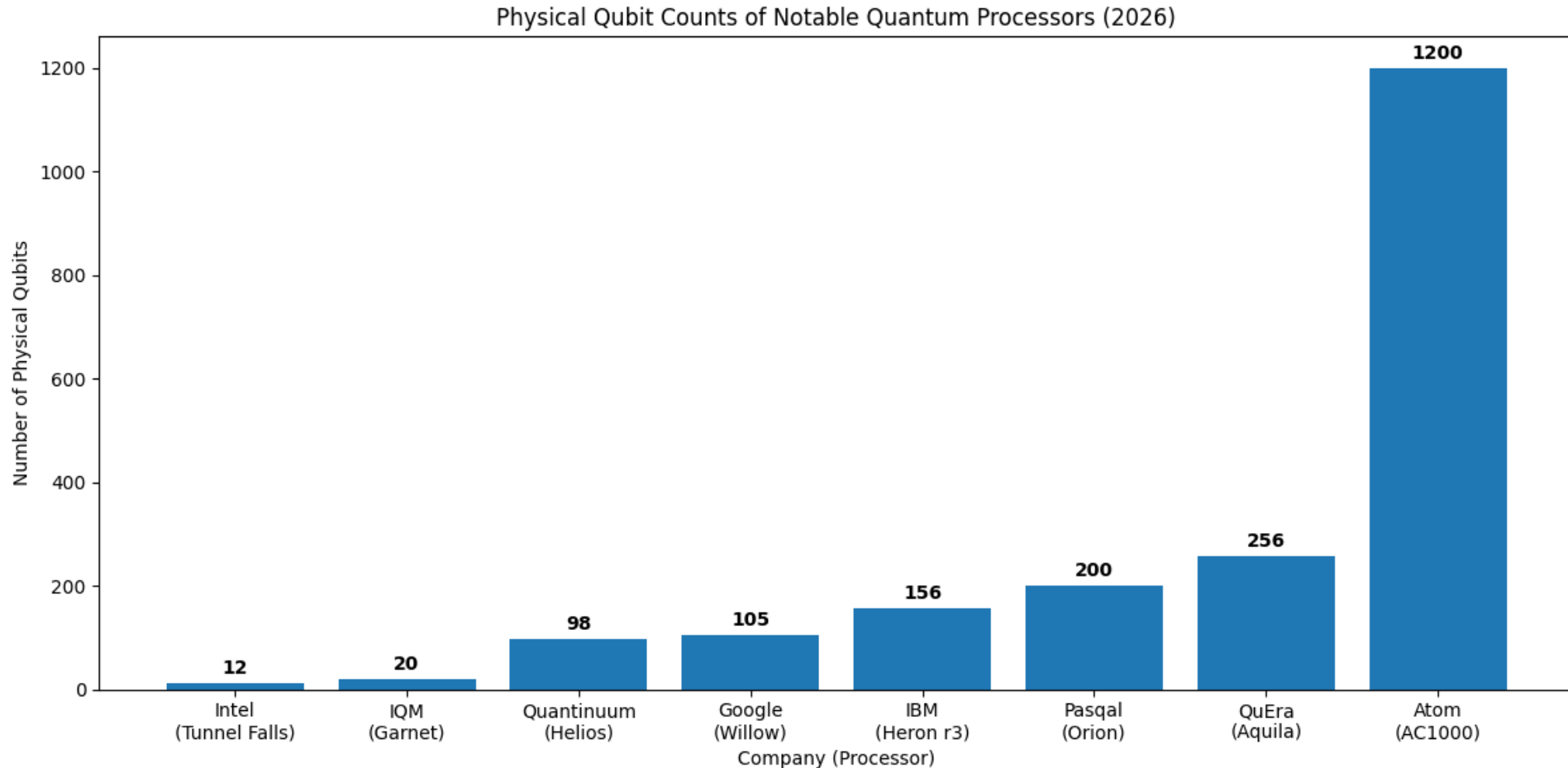
J. M. Gambetta et al. Nature Communications (2017).

1. Intro to quantum computing?



<https://thequantuminsider.com/2026/06/05/how-many-quantum-chip-companies-are-there/>

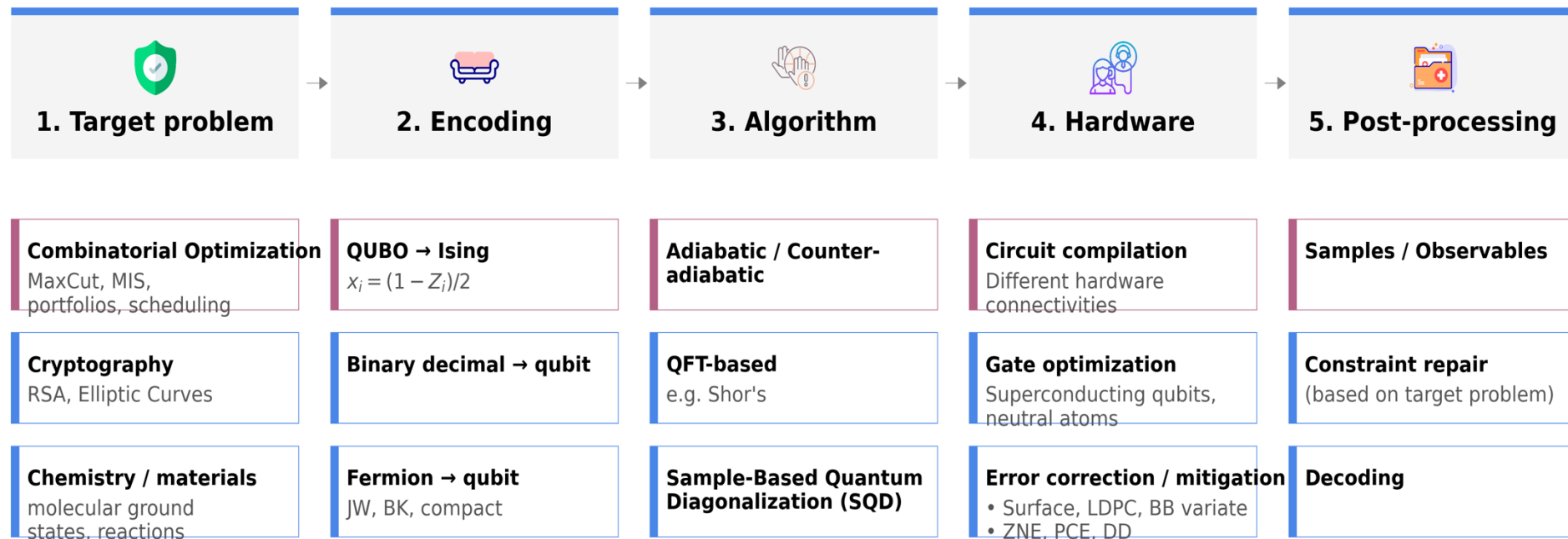
1. Intro to quantum computing?



<https://thequantuminsider.com/2026/06/05/how-many-quantum-chip-companies-are-there/>

1. Intro to quantum computing?

The full pipeline of a quantum solver



1. Intro to quantum computing?

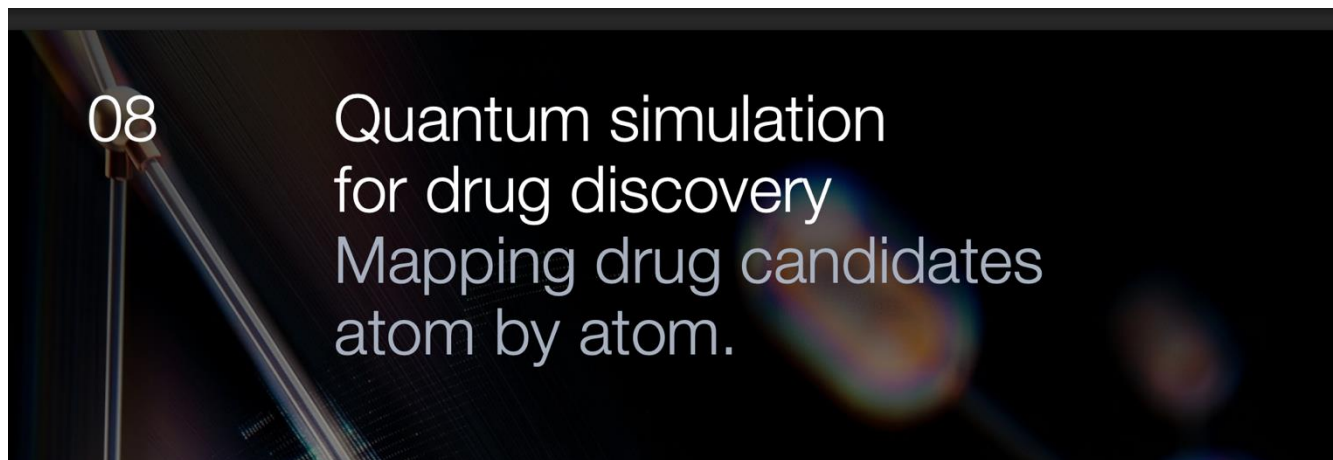
Scott Aaronson
UT Austin

What Will QCs Be Good For?

- Simulating quantum physics and chemistry
- Breaking current public-key encryption
- We'll need to get lucky for most other applications
(The world has often been lied to about this)
- But no matter! The **#1 application**: disproving all the people who say it can never work!

HDMI
1080p 59.8

1. Intro to quantum computing?

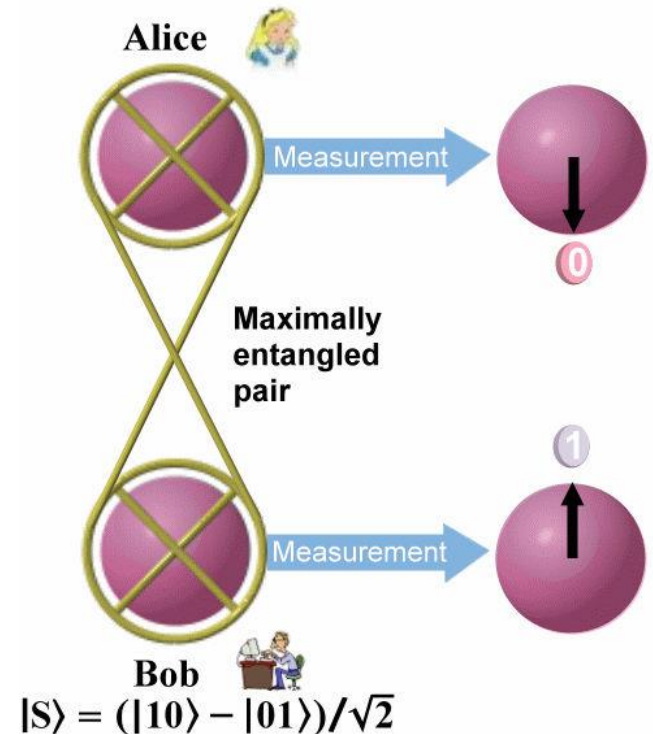
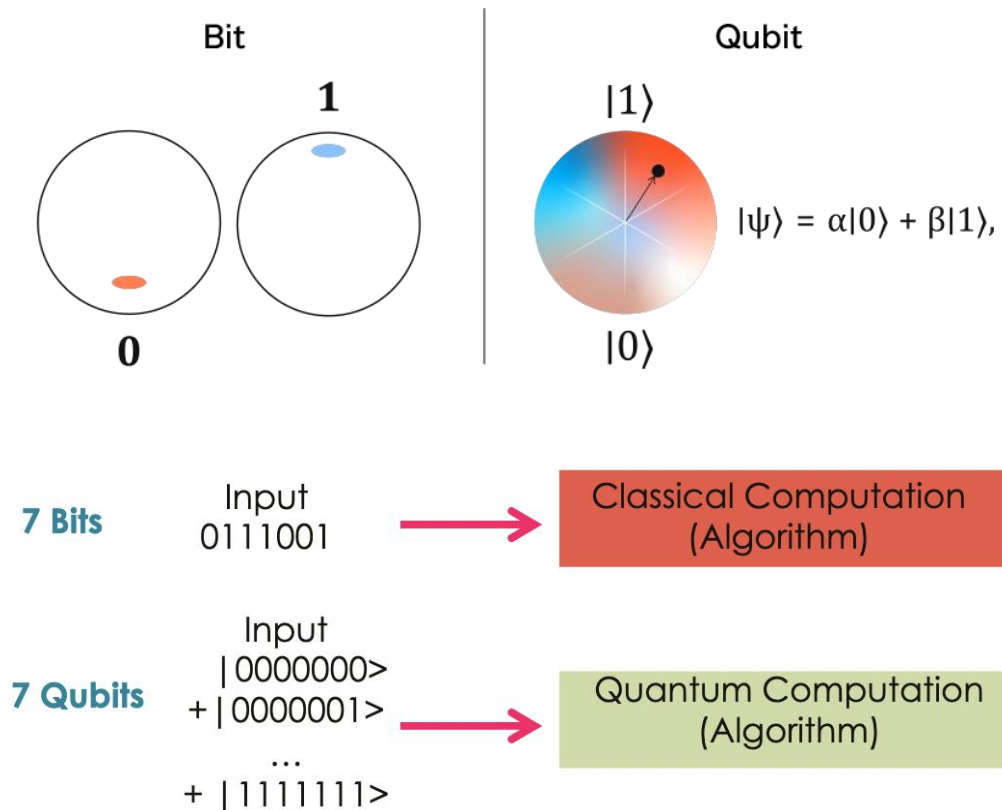


https://reports.weforum.org/docs/WEF_Top_10_Emerging_Technologies_Report_2026.pdf

1. Intro to quantum computing?

Qubits

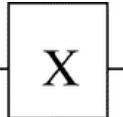
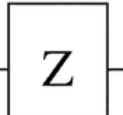
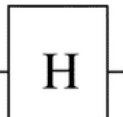
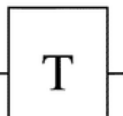
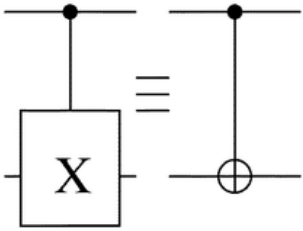
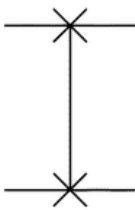
- **Superposition:** A qubit can exist in both 0 and 1 states simultaneously
- **Entanglement:** Two or more qubits can be linked together regardless of distance.



1. Intro to quantum computing?

Quantum gates

unitary matrices

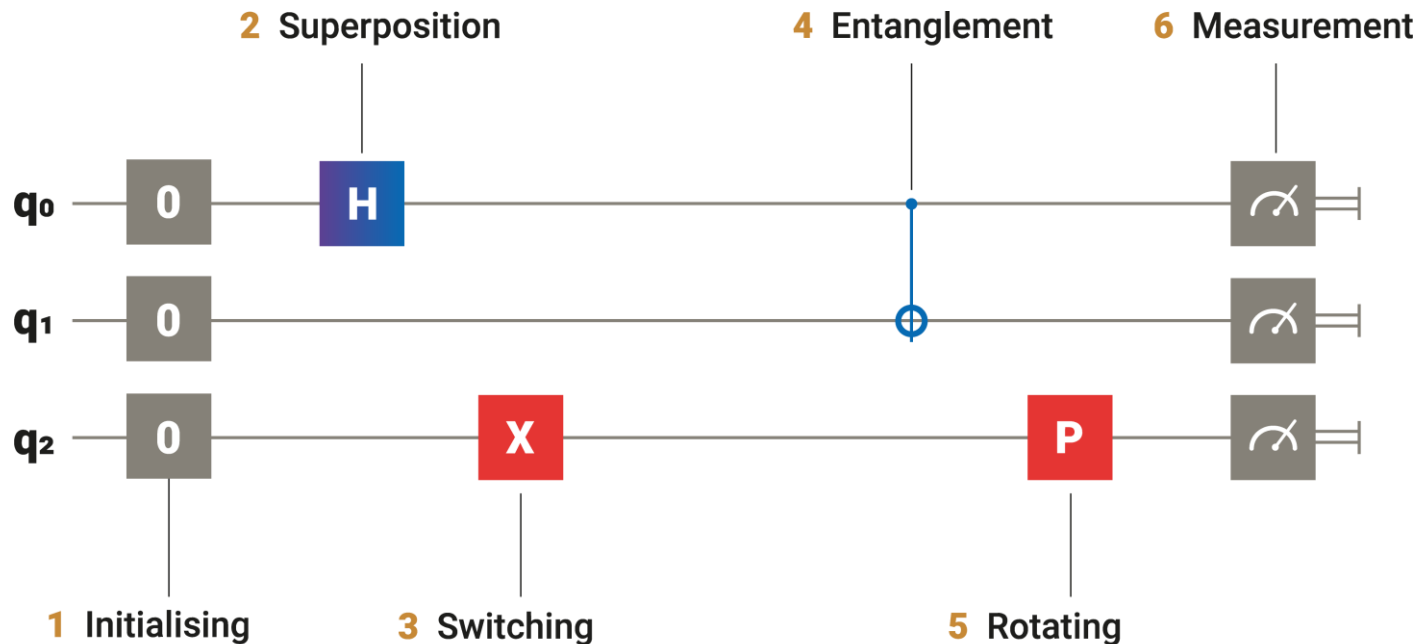
X Gate Bit-flip, Not		$\equiv$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \beta 0\rangle + \alpha 1\rangle$
Z Gate Phase-flip		$\equiv$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha 0\rangle - \beta 1\rangle$
H Gate Hadamard		$\equiv$	$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \frac{\alpha + \beta 0\rangle + \alpha - \beta 1\rangle}{\sqrt{2}}$
T Gate		$\equiv$	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha 0\rangle + e^{i\pi/4}\beta 1\rangle$
Controlled Not Controlled X CNot		$\equiv$	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = a 00\rangle + b 01\rangle + d 10\rangle + c 11\rangle$
Swap		$\equiv$	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = a 00\rangle + c 01\rangle + b 10\rangle + d 11\rangle$

1. Intro to quantum computing?

Quantum circuits

A quantum circuit is the quantum computing equivalent of a classical digital circuit.

A quantum circuit represents a universal set of quantum gates and qubits that perform specific computations.



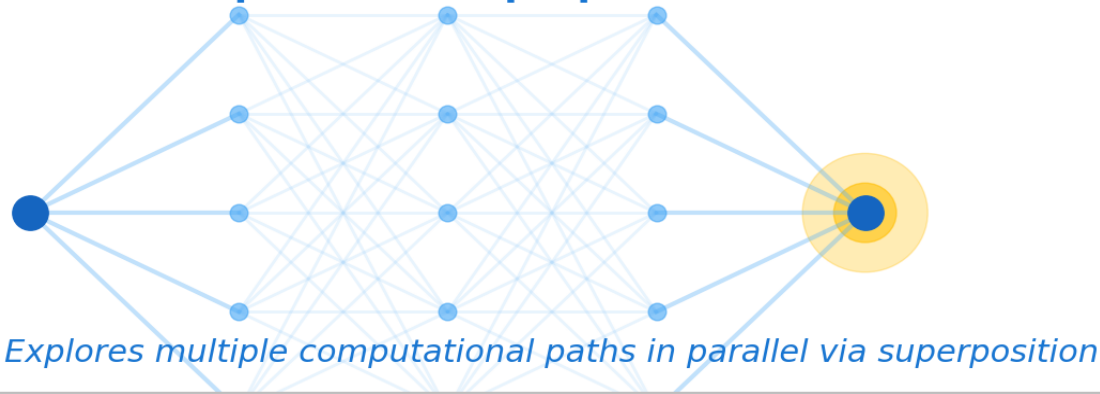
1. Intro to quantum computing?

Conceptualizing Quantum Parallelism

Classical Computation: Sequential Path Exploration



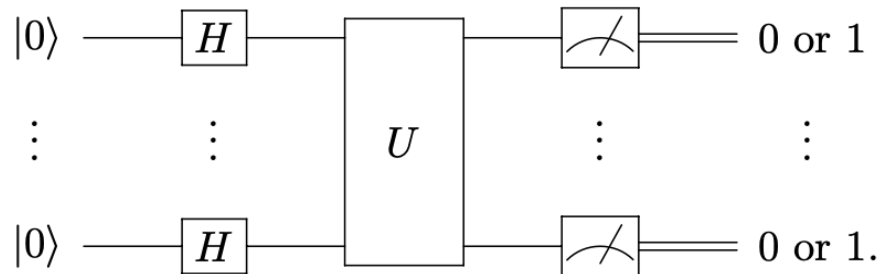
Quantum Computation: Superposition & Interference



Quantum circuits use quantum superposition, which allows multiple computational paths to be explored in parallel. However, this doesn't translate to universal speedups—the advantage applies to specific algorithms where this quantum property can be efficiently harnessed.

1. Intro to quantum computing?

Quantum parallelism



$$(H|0\rangle) \otimes \cdots \otimes (H|0\rangle)$$

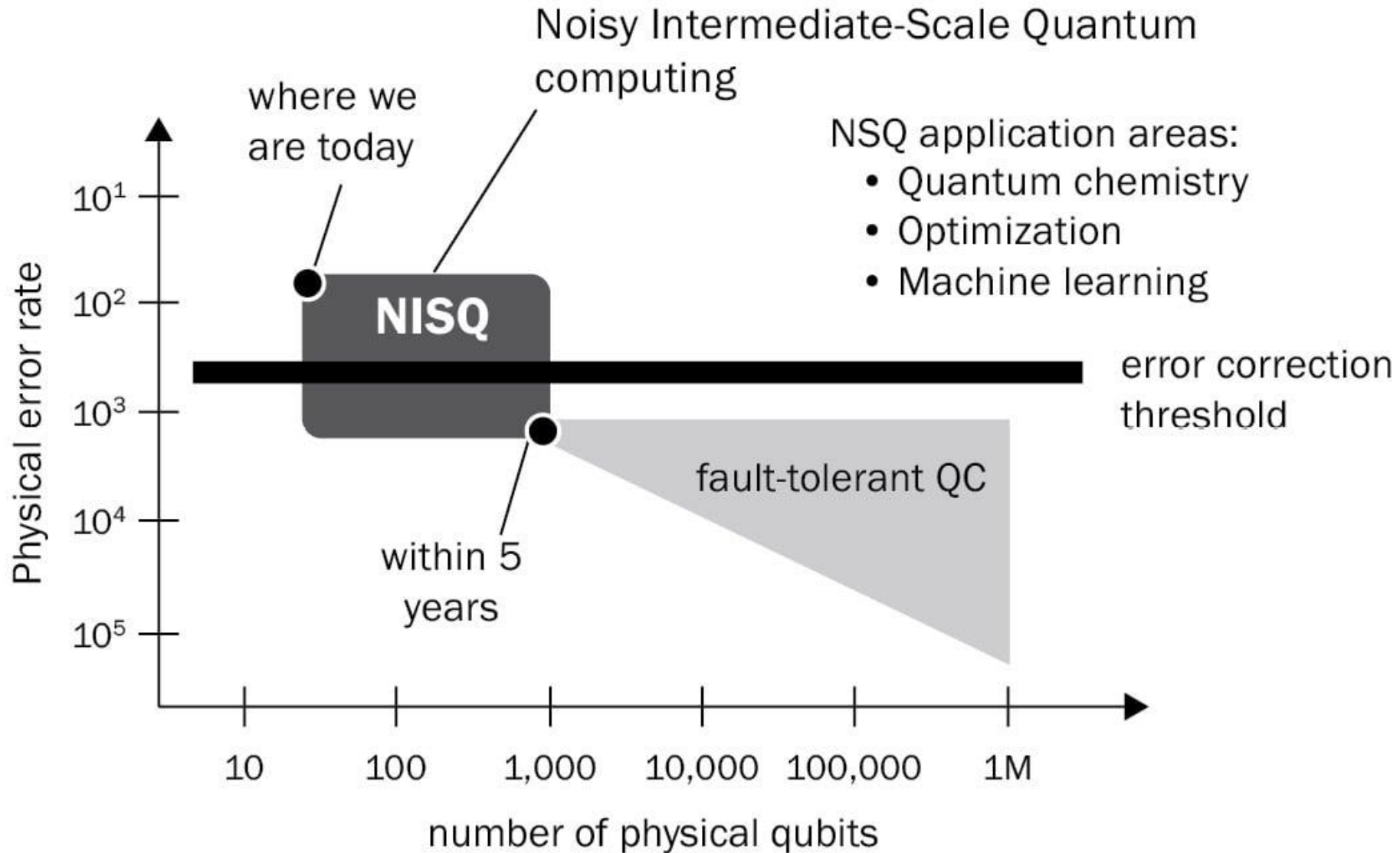
$$\left(\frac{|0\rangle + |1\rangle}{\sqrt{2}} \right) \otimes \cdots \otimes \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}} \right)$$

$$\frac{1}{\sqrt{2^n}} (|0 \cdots 0\rangle + |0 \cdots 01\rangle + |0 \cdots 10\rangle + \cdots + |1 \cdots 1\rangle).$$

n-bit string

- All possible inputs of a classical algorithm are represented by kets in the sum above.
- U is applied to all kets of the sum above simultaneously $\rightarrow$ it is possible to **perform 2^n simultaneous computations** on a n -qubit quantum computer

1. Intro to quantum computing?



1. Intro to quantum computing?

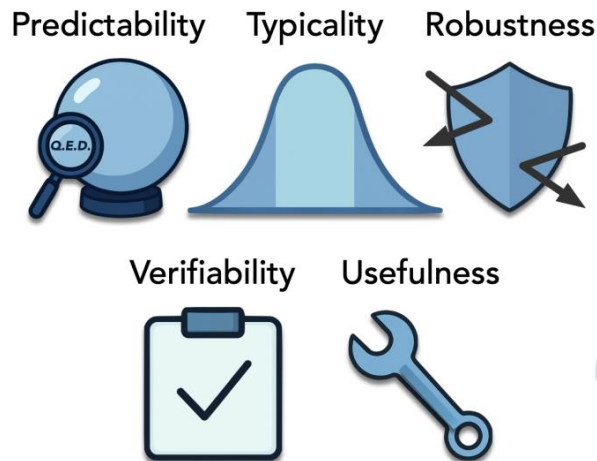
Quantum advantages

Quantum advantage is a demonstrated capability of quantum computers to perform a specific task with superior efficiency, accuracy, or cost-effectiveness compared to the best classical methods, often by leveraging the unique properties of quantum mechanics to solve problems currently intractable for even the most powerful supercomputers.

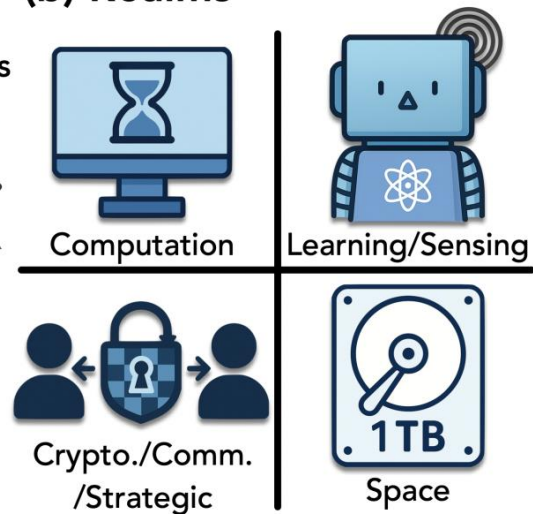


John P. Preskill, CALTECH

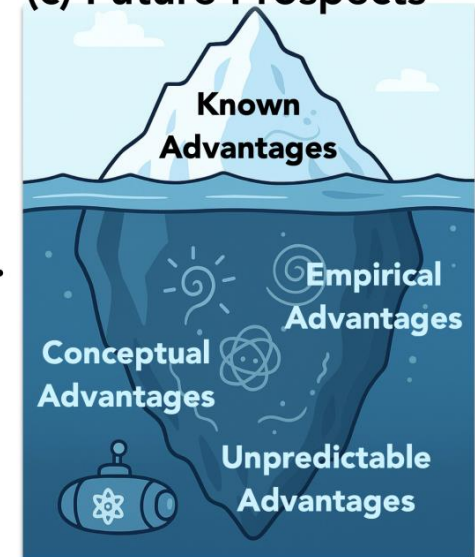
(a) Keystone Properties



(b) Realms



(c) Future Prospects



1. Intro to quantum computing?

Quantum advantages

Predictability. A quantum advantage is predictable if we have sufficient evidence supporting that, given the necessary quantum technology, we will achieve capabilities fundamentally beyond what is possible with classical technology.

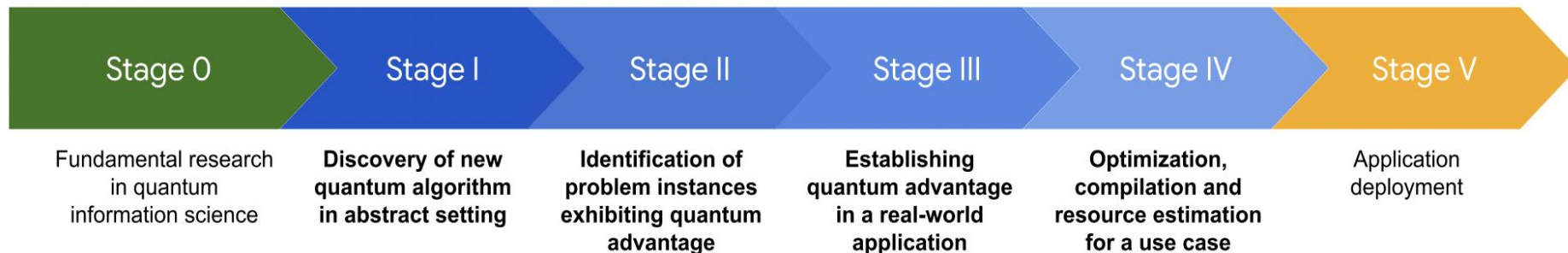
Typicality. A quantum advantage exhibits typicality if it applies to a substantial fraction of practically relevant problem instances, rather than being confined to particular instances that are especially hard classically.

Robustness. A quantum advantage is robust if it persists despite deviations from idealized theoretical assumptions, including imperfections in hardware, available resources, input data, etc

PHYS. REV. X 16, 030501 (2026)

For benchmarks
without application

PRX QUANTUM 7, 020101 (2026)



1. Intro to quantum computing?

Quantum advantages

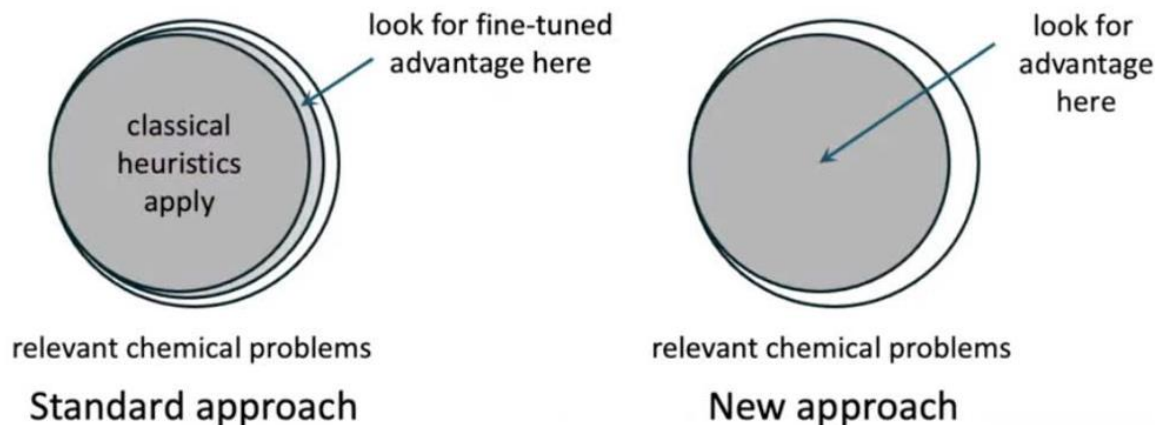


Garnet Chan,
Caltech

A different view on quantum advantage

Don't look for quantum advantage by hoping for classical "intractability"

Find quantum advantage where classical heuristic assumptions can be applied!



Can we achieve quantum speedups under classical heuristic assumptions?

1. Intro to quantum computing?

nature communications



Article

<https://doi.org/10.1038/s41467-023-37587-6>

Evaluating the evidence for exponential quantum advantage in ground-state quantum chemistry

**Hope but
not hype!**

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Published online: 07 April 2023

Check for updates

Seunghoon Lee¹, Joonho Lee², Huanchen Zhai¹, Yu Tong³, Alexander M. Dalzell⁴, Ashutosh Kumar^{5,6}, Phillip Helms¹, Johnnie Gray¹, Zhi-Hao Cui¹, Wenyuan Liu¹, Michael Kastoryano^{4,7}, Ryan Babbush⁸, John Preskill^{4,9}, David R. Reichman², Earl T. Campbell¹⁰, Edward F. Valeev⁵, Lin Lin^{3,11} & Garnet Kin-Lic Chan¹✉

“Quantum computing can model molecular interactions for drug discovery and analyze complex health datasets, **but better hardware is needed.**”

CAN QUANTUM COMPUTING CRACK THE BIGGEST CHALLENGES IN HEALTH?

Quantum computing can model molecular interactions for drug discovery and analyze complex health datasets, but better hardware is needed. **By Marianne Guenot**

Cleveland Clinic in the USA and the UK National Health Service are both part of a burgeoning community of researchers, health systems and companies exploring applications of quantum computing in health. Although this nascent technology is at least a few years away from having practical

applications – and some are warning of the impending burst of the ‘quantum bubble’ – many experts believe that biomedical and healthcare research needs to be ready for the quantum revolution of tomorrow.

“I know we are taking a gamble,” says Lara Jehi, Cleveland Clinic’s chief research information officer, who leads the institute’s

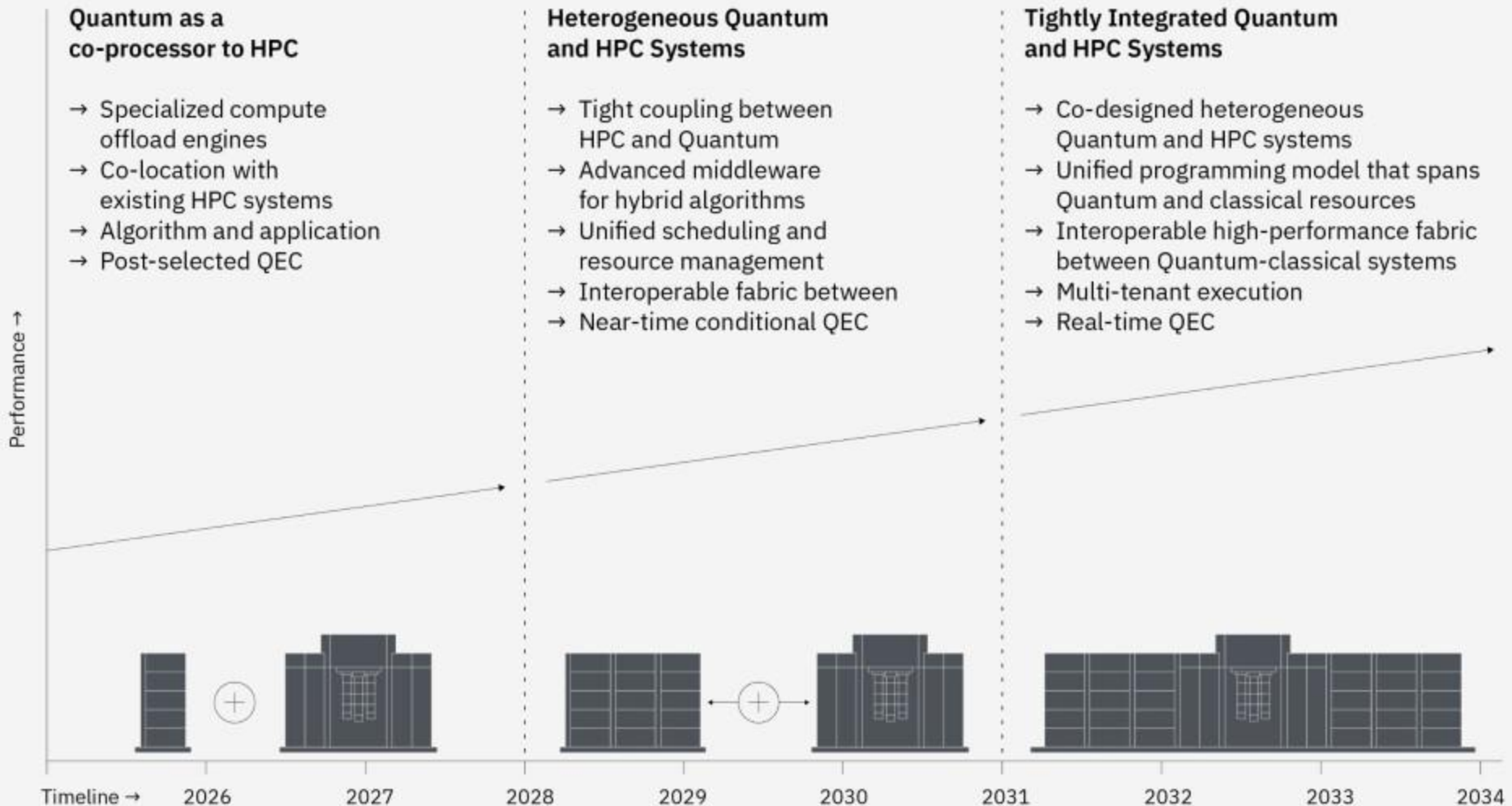
quantum research. Jehi hopes that “there is a strategic, long-term advantage in being the group that was first.”

Health applications

Since last year, those grabbing food at the Cleveland Clinic medical research center cafeteria have had an odd companion at the

1. Intro to quantum computing?

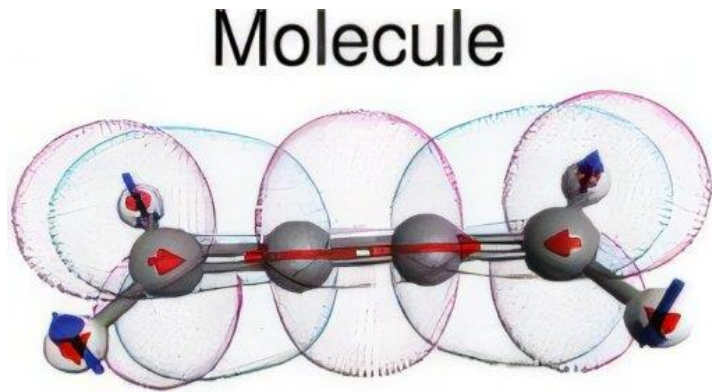
IBM's strategy: Quantum centric supercomputing



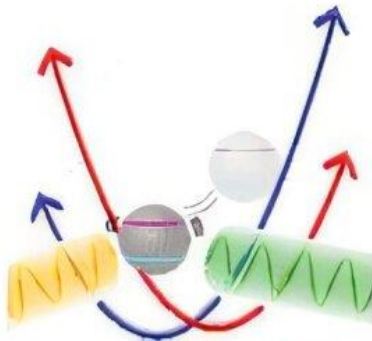
Outline

1. What is Quantum computing (QC)?
- 2. Quantum many-body simulation**
3. Quantum optimization
4. Quantum machine learning
5. Summary

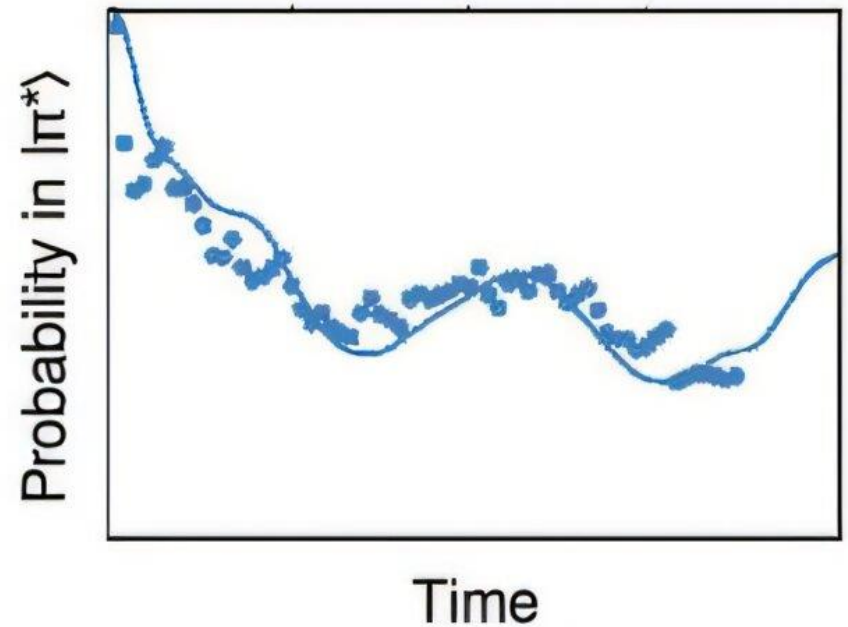
2. Quantum many-body simulation



Quantum simulator



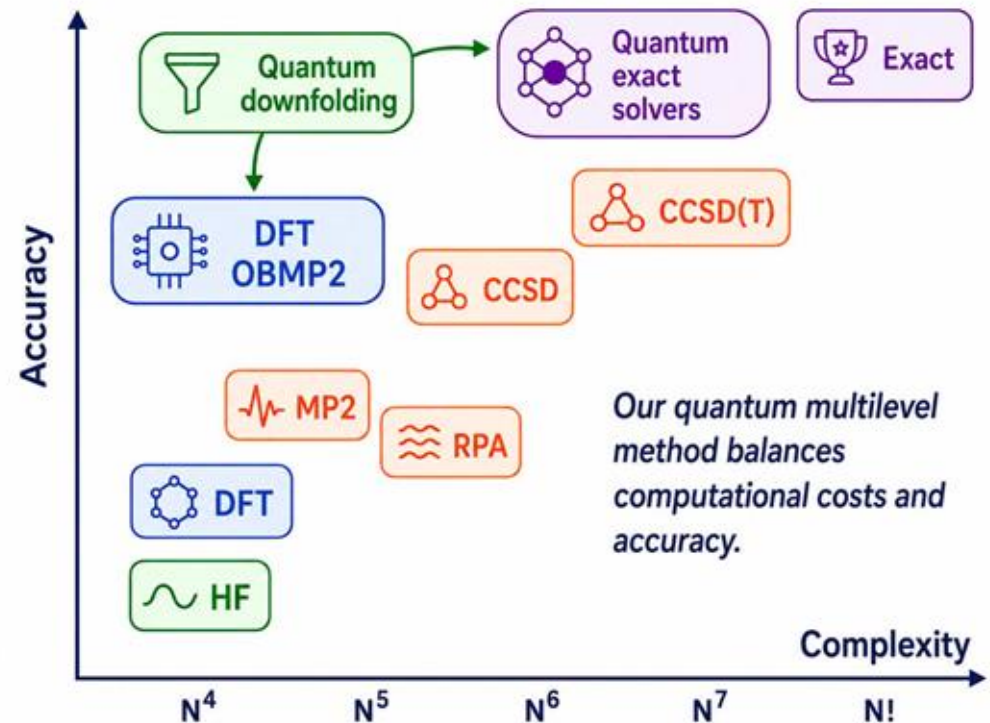
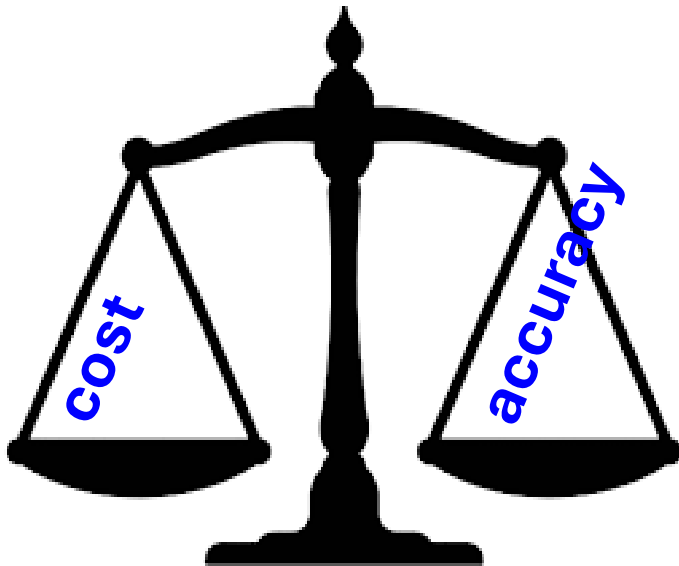
$$i\hbar \frac{\partial \psi}{\partial t} = \underbrace{-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}}_{\text{K.E.}} + \underbrace{V \cdot \psi}_{\text{P.E.}}$$



2. Quantum many-body simulation

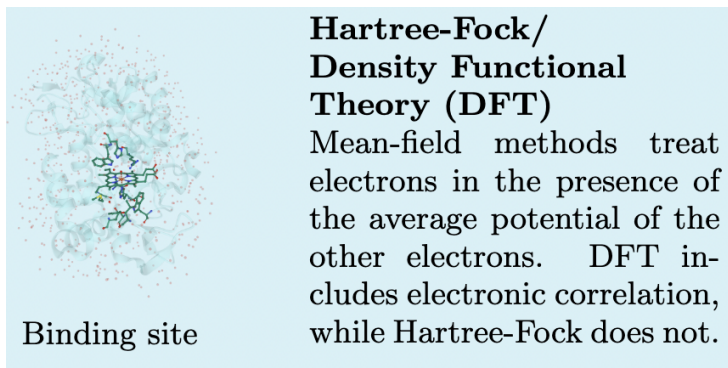
- In the Born-Oppenheimer approximation, molecular electronic Hamiltonian has form:

$$H_e = -\sum_i \frac{\nabla_i^2}{2} - \sum_{i,I} \frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}.$$



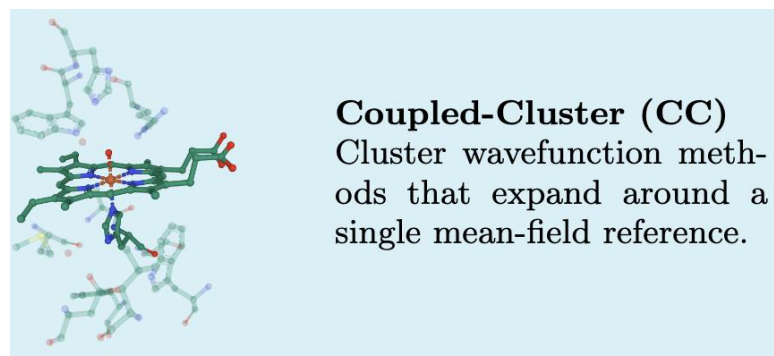
2. Quantum many-body simulation

$O(N^4)$

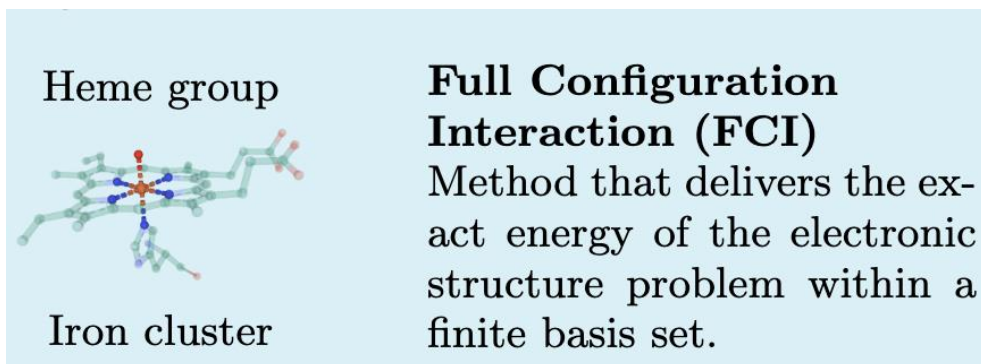


**Quantum computing is
expected to solve problems
intractable for “classical”
ab-initio methods!**

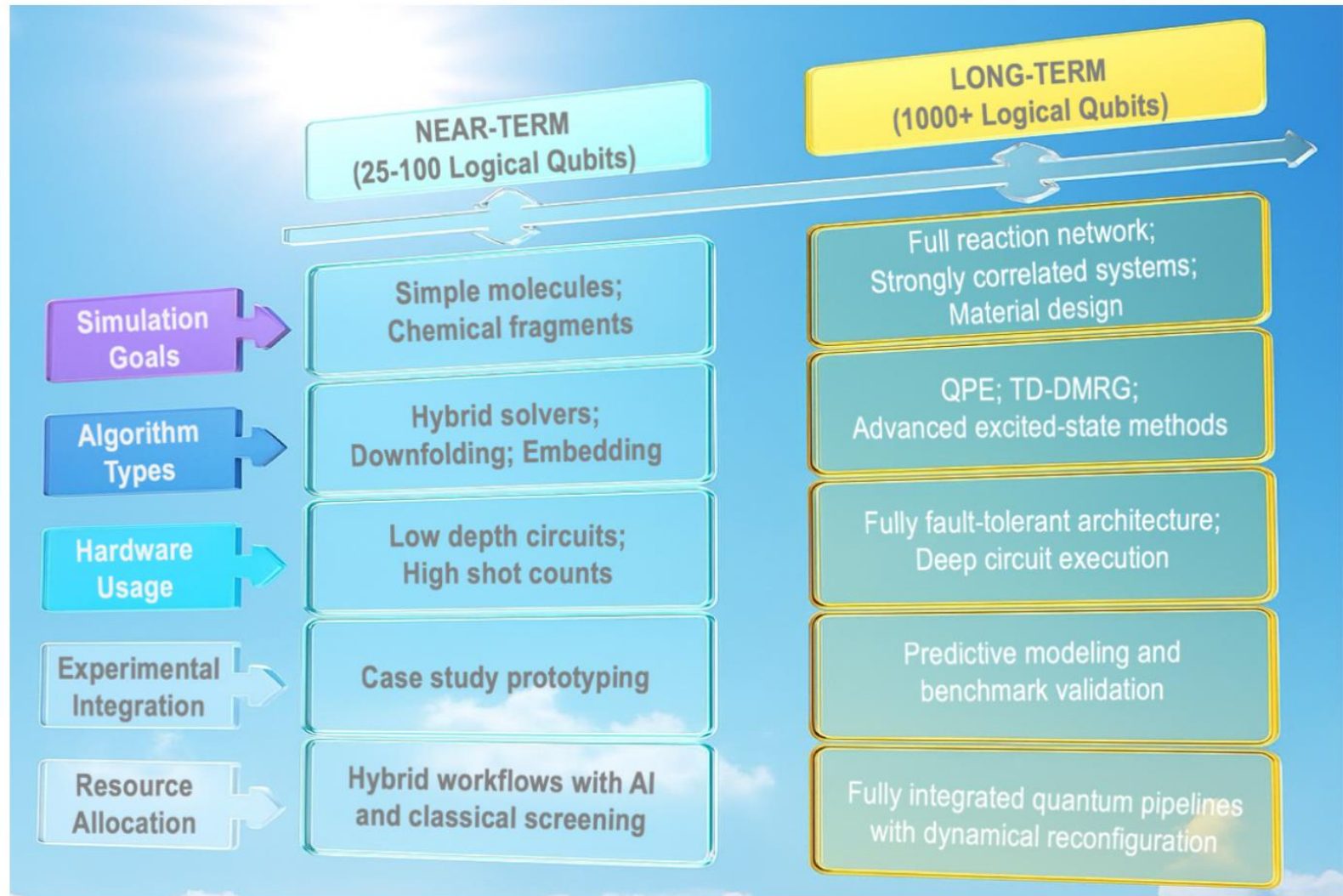
$O(N^7)$



Exponential!



2. Quantum many-body simulation



2. Quantum many-body simulation

Mapping from fermions to qubit

The JW mapping encodes the electronic wavefunction in an array of qubits by mapping the occupation number of spin orbitals in qubits.

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The occupation number of n spin orbitals is stored in N qubits.

$|0\rangle_j$ corresponds to the j^{th} spin orbital being unoccupied

$|1\rangle_j$ corresponds to the j^{th} spin orbital being occupied

$$\hat{a}_j^\dagger \xrightarrow{?} |1\rangle\langle 0|_j = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} = \frac{X_j - iY_j}{2}$$
$$\hat{a}_j \xrightarrow{?} |0\rangle\langle 1|_j = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} = \frac{X_j + iY_j}{2},$$

These do not maintain the anti-commutation of fermionic operators

2. Quantum many-body simulation

Mapping from fermions to qubit

To maintain the anti-commutation, one can include a string of Z operators $Z_0 \otimes \cdots \otimes Z_{j-1}$ acting on each of the other qubits up to the j^{th} .

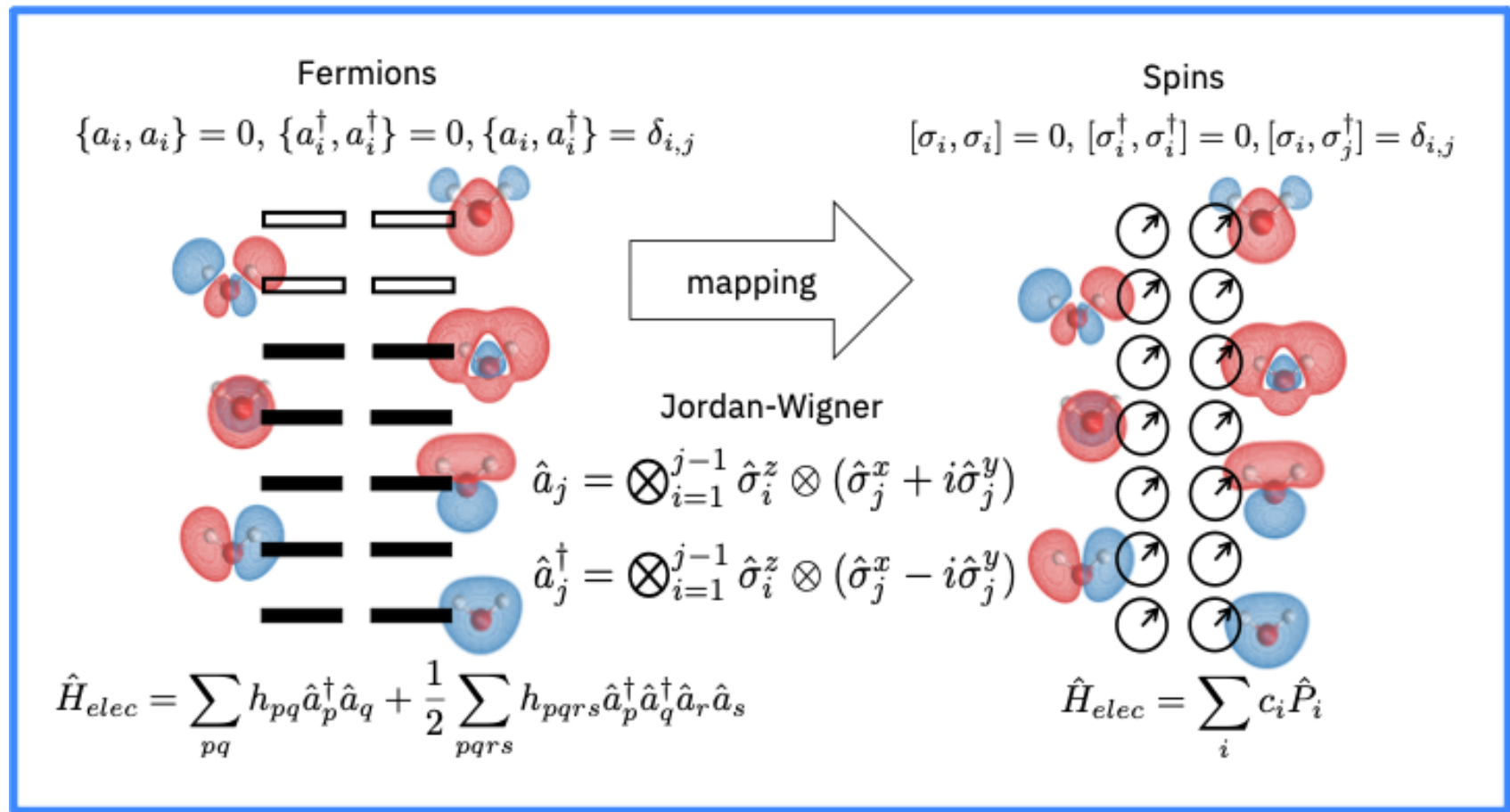
We have that $Z_0 \otimes \cdots \otimes Z_{j-1}$ has eigenvalue $+1$ for states with an even number of occupied orbitals up to the j^{th} , and eigenvalue -1 for states with an odd number of occupied orbitals up to the j^{th} .

JW transform:

$$\begin{aligned} \hat{a}_j^\dagger &\rightarrow \frac{X_j - iY_j}{2} \otimes Z_0 \otimes \cdots \otimes Z_{j-1} \\ \hat{a}_j &\rightarrow \frac{X_j + iY_j}{2} \otimes Z_0 \otimes \cdots \otimes Z_{j-1}. \end{aligned} \quad \longrightarrow \quad \hat{a}_i \hat{a}_j^\dagger = -\hat{a}_j^\dagger \hat{a}_i,$$

2. Quantum many-body simulation

Mapping from fermions to qubit

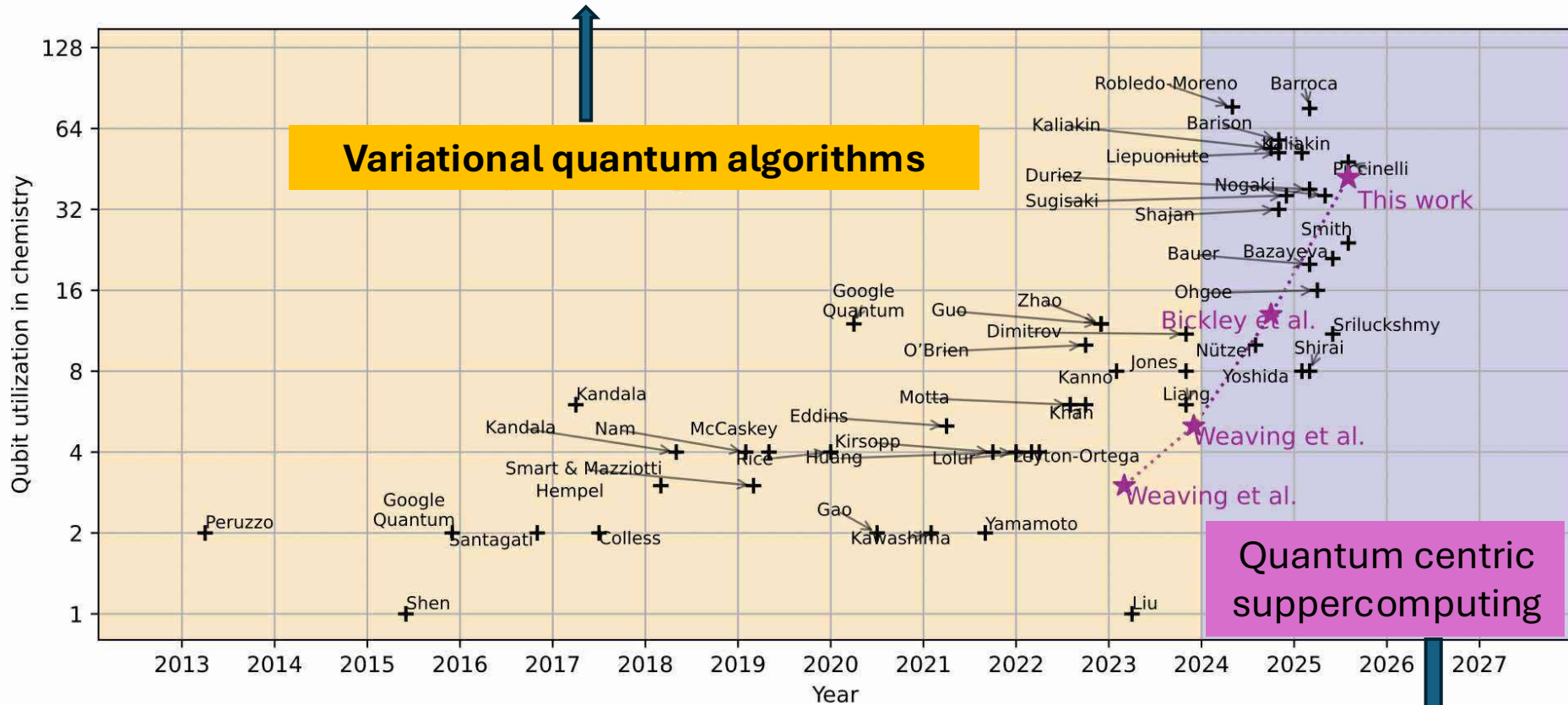


https://qiskit-community.github.io/qiskit-nature/tutorials/06_qubit_mappers.html

2. Quantum many-body simulation

Quantum computing solvers

- Quantum computers measure cost functions
- Classical computers optimize cost functions



- Quantum computers sample states' space
- Classical computers diagonalize Hamiltonian matrix

2. Quantum many-body simulation

- **Variational quantum eigensolver (VQE)** is widely-used
- **VQE** is a classical-quantum hybrid algorithm
- **VQE** lies on the variational principle

$$E_0 \leq \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} \quad \Rightarrow \quad E_{\text{VQE}} = \min_{\theta} \langle \mathbf{0} | U^\dagger(\theta) \hat{H} U(\theta) | \mathbf{0} \rangle$$



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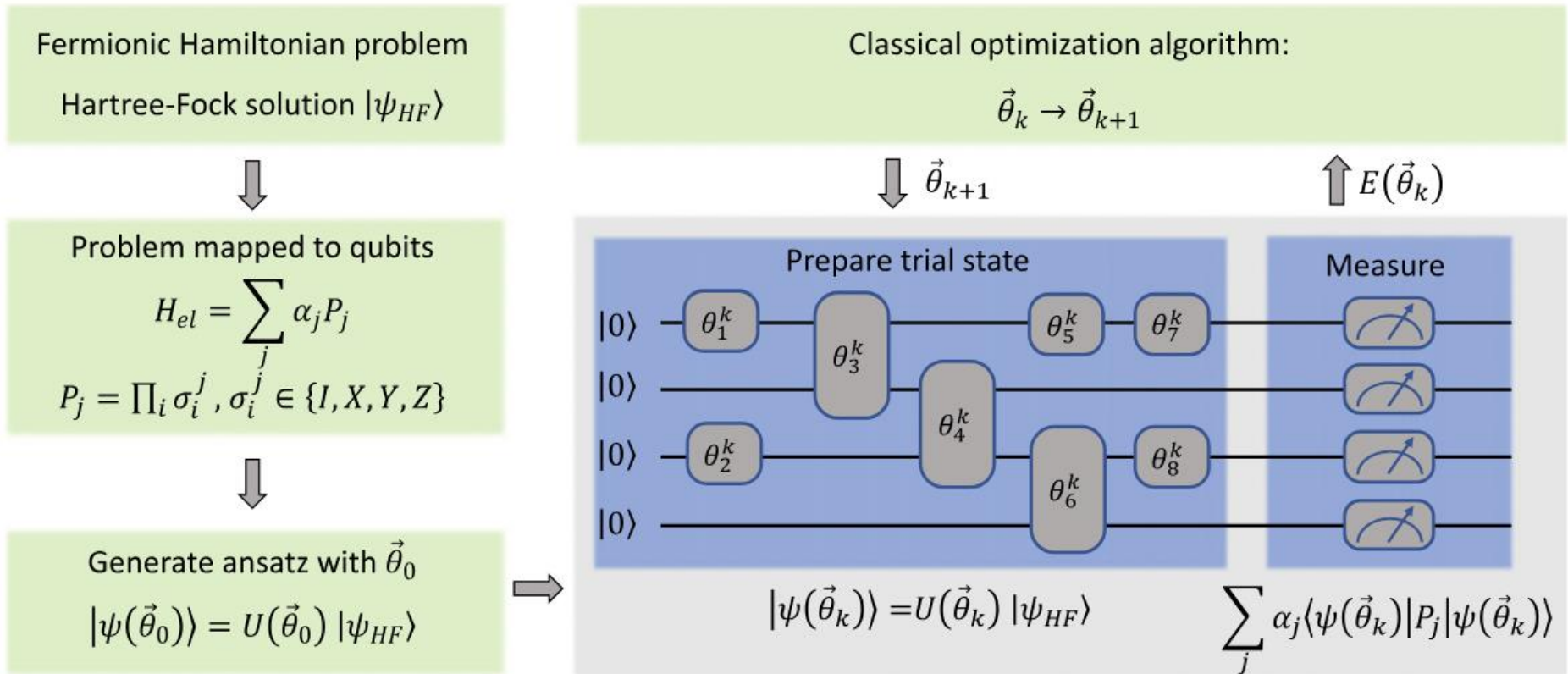
The Variational Quantum Eigensolver: A review of methods and best practices

Jules Tilly^{a,b,*}, Hongxiang Chen^{b,c}, Shuxiang Cao^{b,d}, Dario Picozzi^{a,b},
Kanav Setia^e, Ying Li^f, Edward Grant^{b,c}, Leonard Wossnig^{b,c}, Ivan Rungger^g,
George H. Booth^h, Jonathan Tennyson^a



2. Quantum many-body simulation

VQE: general scheme

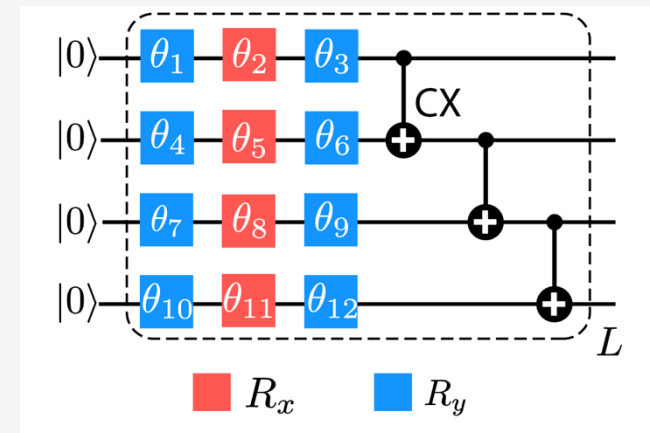


2. Quantum many-body simulation

Ansatz

Listing 1: Simple hardware-efficient ansatz in Python

```
1 from qiskit import QuantumCircuit
2 from qiskit.circuit import ParameterVector
3
4 def create_heal(n_qubits, n_layers):
5     qc = QuantumCircuit(n_qubits)
6     theta = ParameterVector("theta", length=2 * n_qubits * n_layers)
7
8     p = 0
9     for l in range(n_layers):
10         # Rotation layer
11         for q in range(n_qubits):
12             qc.ry(theta[p], q)
13             p += 1
14             qc.rz(theta[p], q)
15             p += 1
16
17         # Entangling layer
18         for q in range(n_qubits - 1):
19             qc.cx(q, q + 1)
20
21     return qc
22
23 qc = create_heal(4, 2)
24 print(qc.draw())
```



2. Quantum many-body simulation

Cost function

In many cases, the cost function $C(\theta)$ is defined as an expectation value of

$$C(\theta) = \langle \psi(\theta) | \hat{O} | \psi(\theta) \rangle,$$

where:

- θ is the vector of parameters (such as gate rotation angles) that define the quantum state or quantum circuit.
- $|\psi(\theta)\rangle$ is the quantum state prepared by the quantum circuit with parameters θ .
- $\hat{O}$ is an observable, which is a Hermitian operator that represents the quantity we want to measure or optimize.

$$\begin{aligned} C(\theta) &= \sum_n c_n \langle \psi(\theta) | n \rangle \langle n | \psi(\theta) \rangle \\ &= \sum_n c_n |\langle n | \psi(\theta) \rangle|^2 \\ &= \sum_n c_n p(n) \end{aligned}$$

2. Quantum many-body simulation

Gradient: parameter-shift rule

- Consider a parameterized gate $U(\theta) = e^{-i\theta G}$ where G is the generator, O is the measured observable and ψ is the initial state:

$$C(\theta) = \langle \psi | U^\dagger O U | \psi \rangle$$

- The derivative w.r.t the parameter θ yields:

$$\frac{\partial}{\partial \theta} C(\theta) = -i \langle \psi | U^\dagger(\theta) [O, G] U(\theta) | \psi \rangle$$

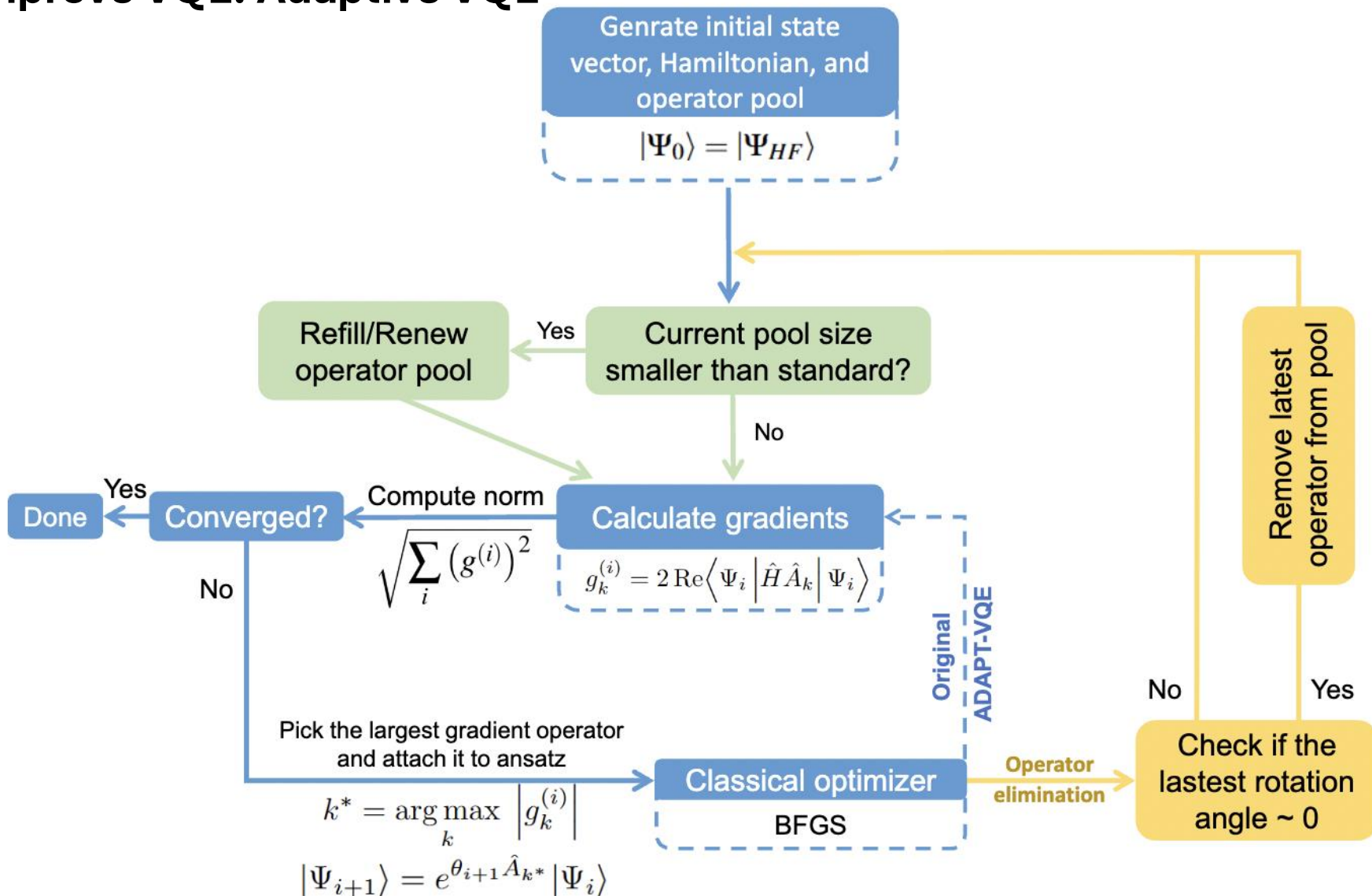
$$|\psi\rangle \rightarrow \boxed{U(\theta + s)} \rightarrow \boxed{\text{meter}} \rightarrow C(\theta + s)$$

$$|\psi\rangle \rightarrow \boxed{U(\theta - s)} \rightarrow \boxed{\text{meter}} \rightarrow C(\theta - s)$$

$$\frac{\partial}{\partial \theta} C(\theta) = \frac{1}{2 \sin(s)} [C(\theta + s) - C(\theta - s)]$$

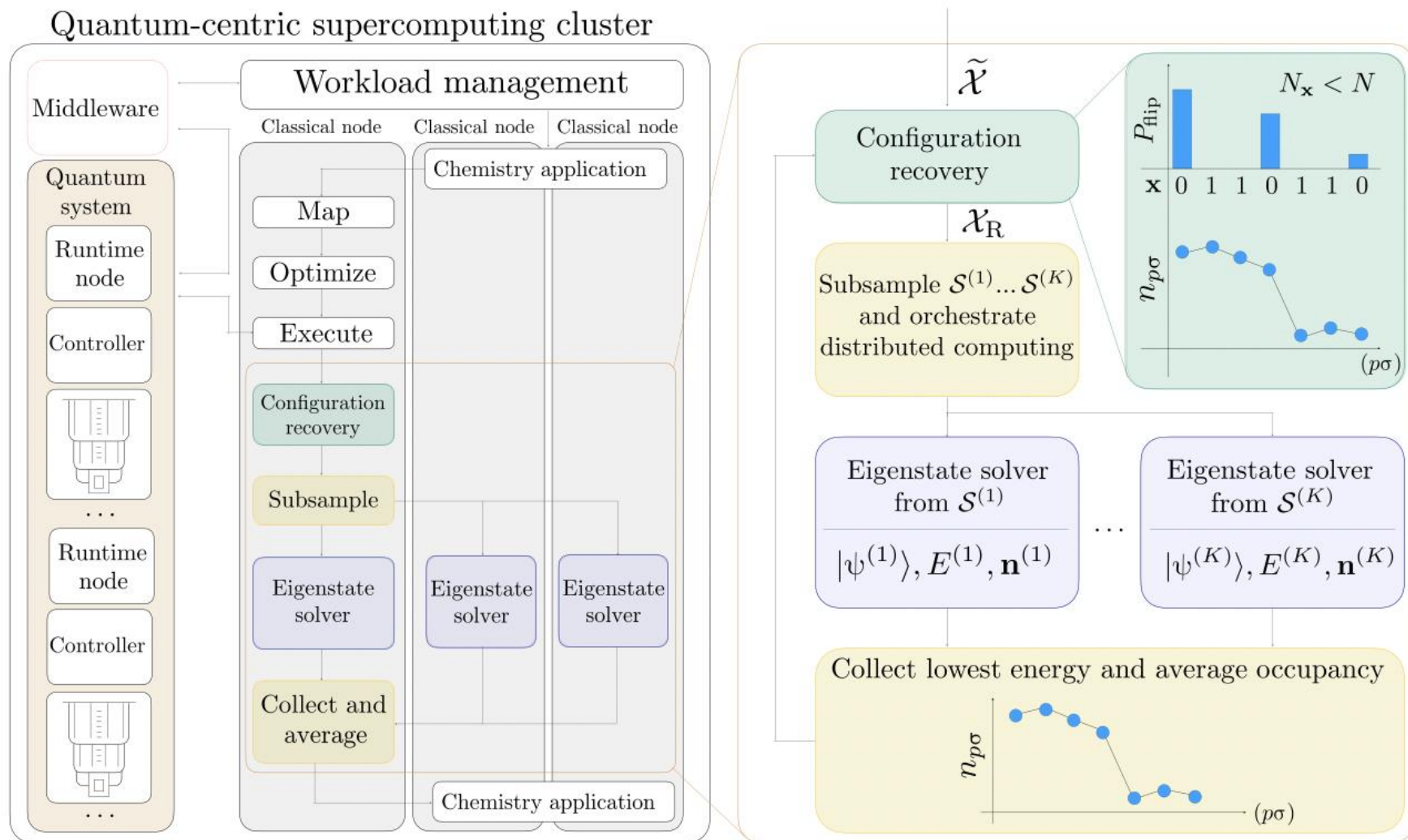
2. Quantum many-body simulation

Improve VQE: Adaptive VQE



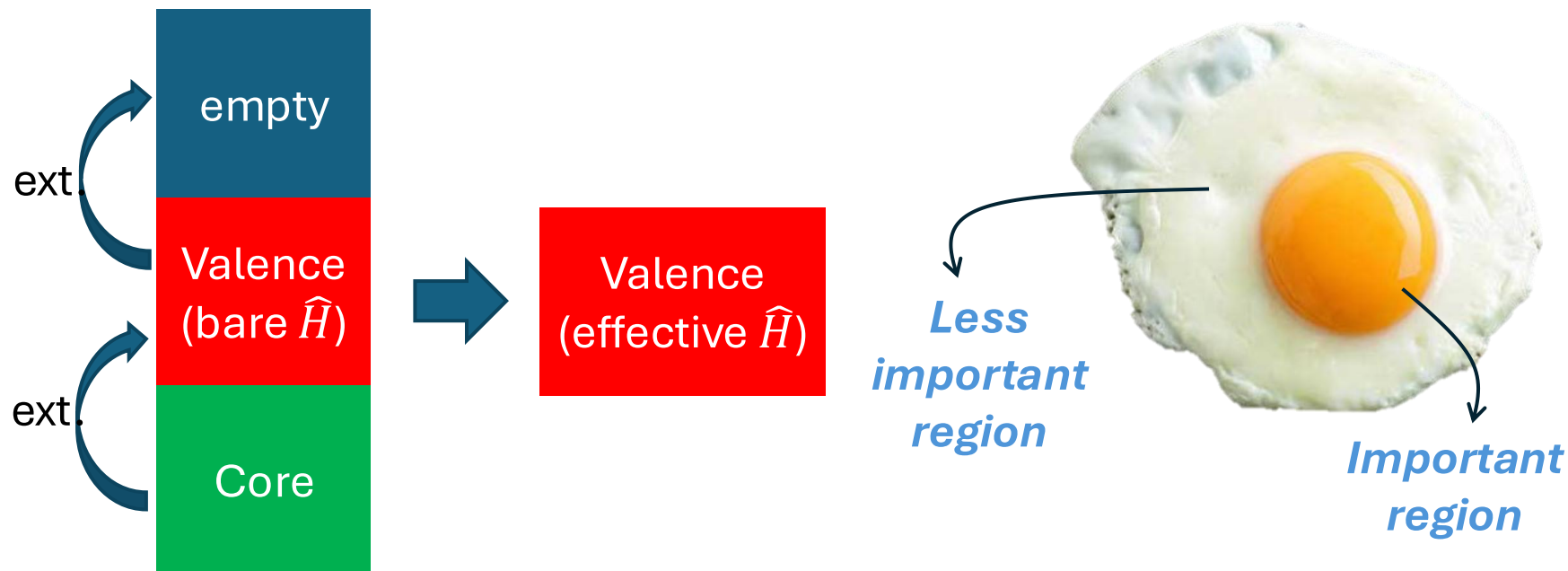
2. Quantum many-body simulation

Sample-based quantum diagonalization (SQD)



2. Quantum many-body simulation

Space reduction: quantum downfolding



TNL, *J Phys Chem A* 2021, **125** 9242

TNL, *Phys Chem Chem Phys* 2022, **24** 19393

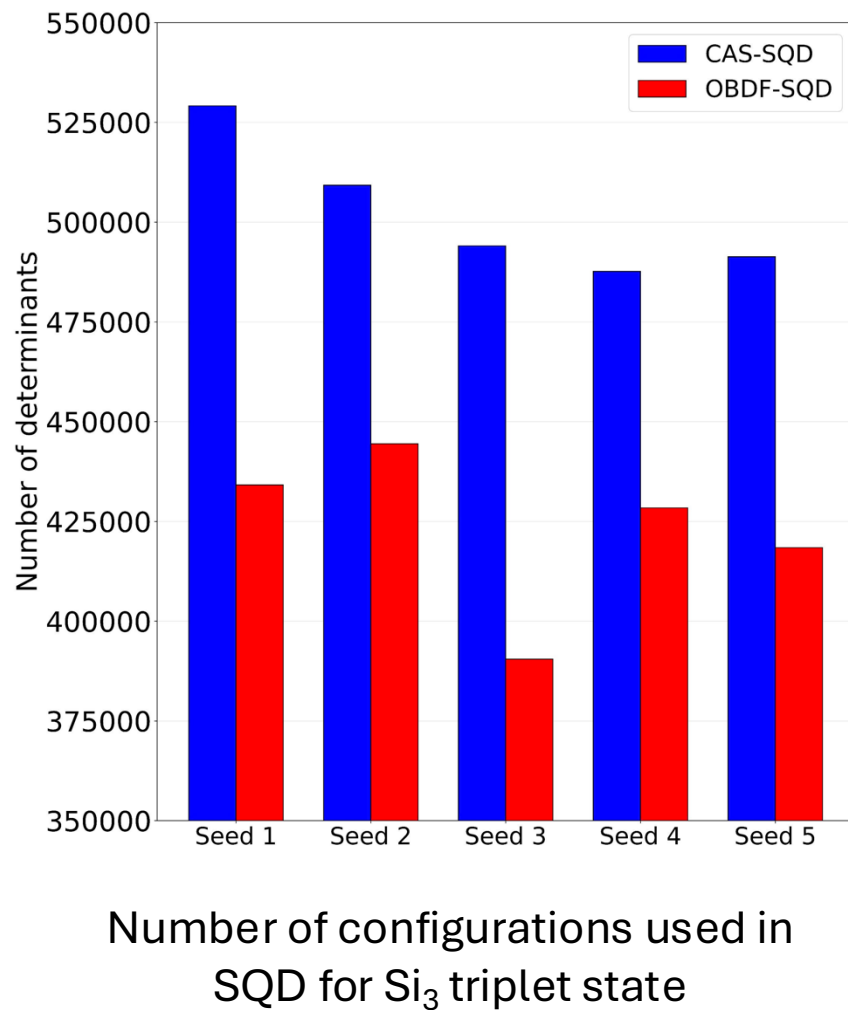
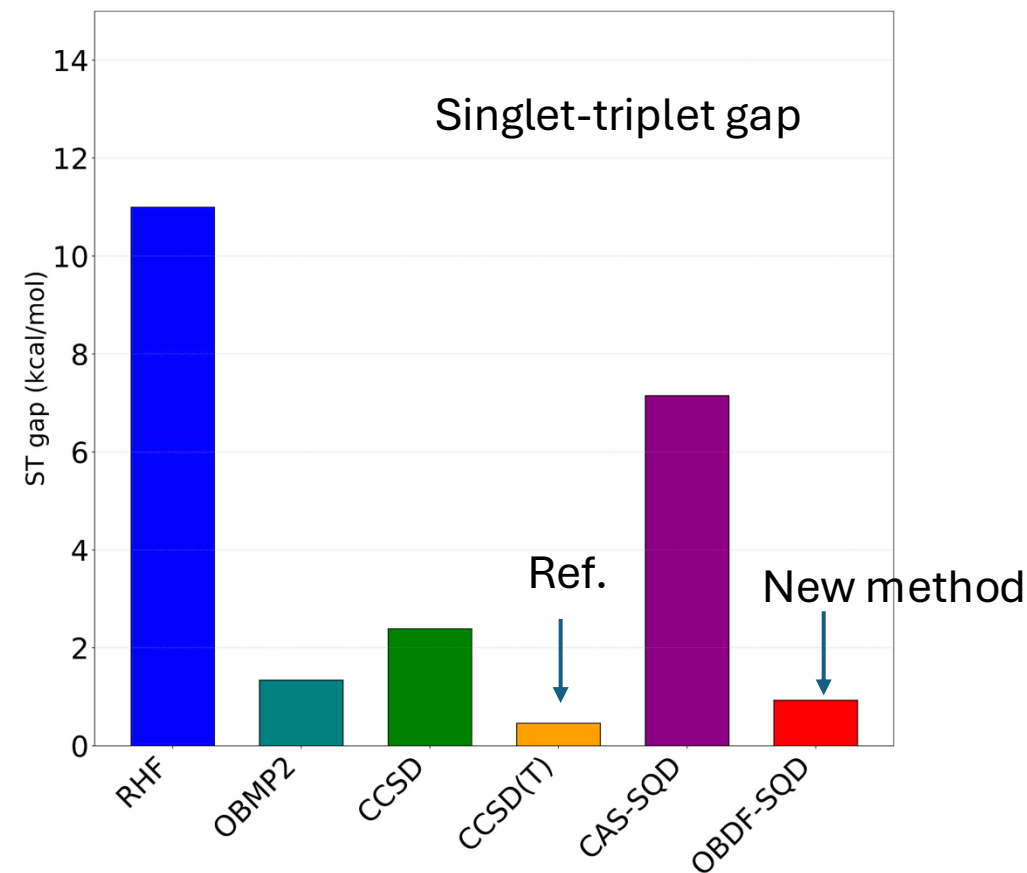
Nhan and **TNL** *J. Phys. Chem. A* 2023 127, 5222

Nhan, Hoang and **TNL**, *J Phys Chem A* 2024 128 (8), 1543

Nhan and **TNL**, *J. Chem. Phys.* 2025 **162**, 104109

2. Quantum many-body simulation

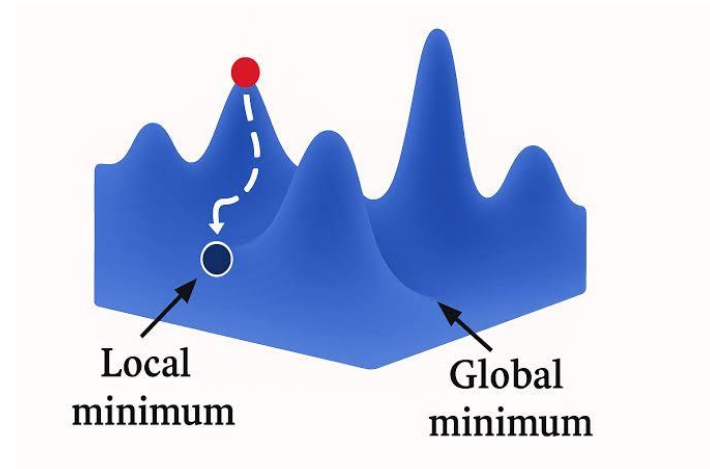
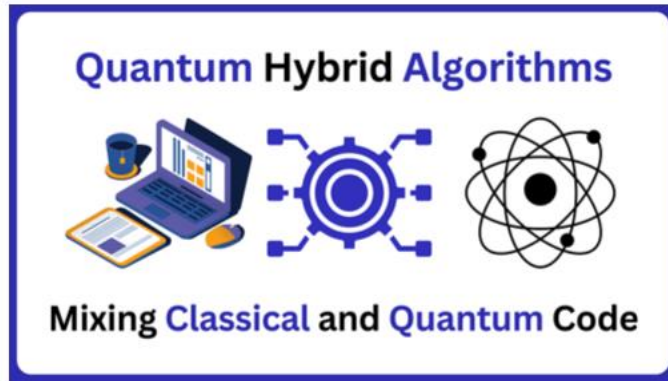
Numerical example: Si_3



Outline

1. What is Quantum computing (QC)?
2. Quantum many-body simulation
- 3. Quantum optimization**
4. Quantum machine learning
5. Summary

3. Quantum optimization



Expected Advantages

- **Simultaneous Exploration:** Superposition lets qubits represent numerous combinations at once, avoiding the sequential bottleneck of classical computers.
- **Quantum Tunneling:** Algorithms pass straight through high energy barriers instead of climbing over them, escaping local minimum traps.
- **Interference Amplification:** Wave interference highlights optimal pathways while muting incorrect options.
- **Hybrid Efficiency:** Modern setups blend classical loops with quantum processing to yield practical gains on current hardware

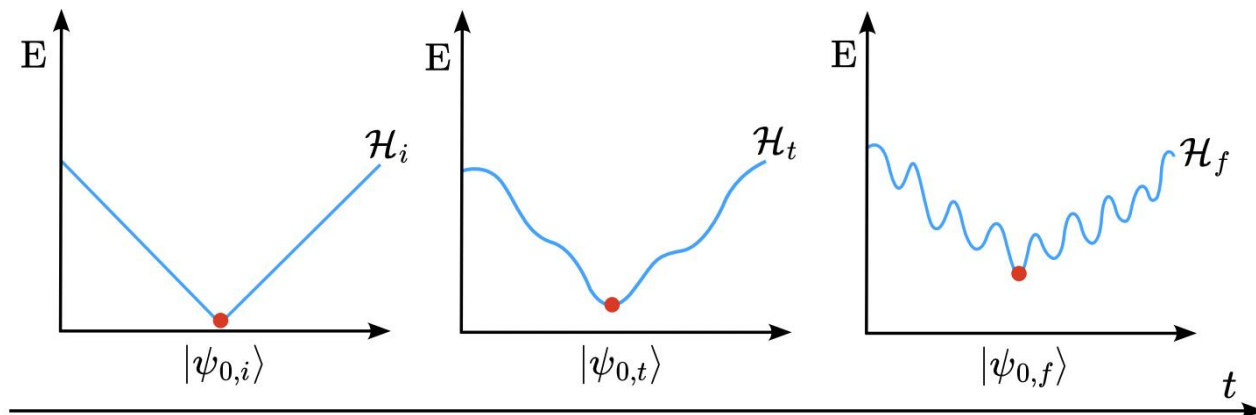
3. Quantum optimization

Quantum Approximate Optimization Algorithm (QAOA)

QAOA operates by iteratively applying two Hamiltonians:

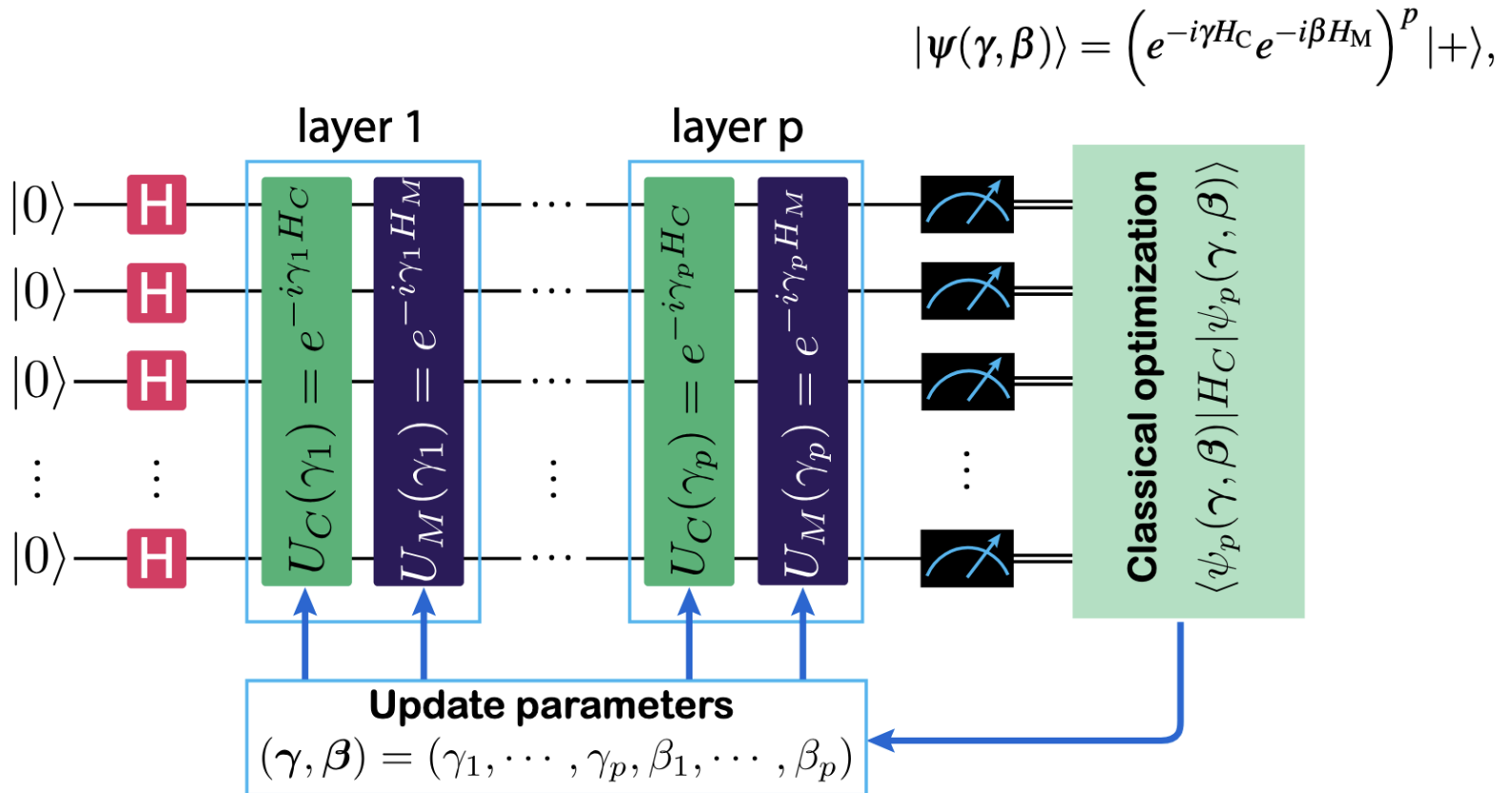
- Cost Hamiltonian (H_C): Encodes the optimization problem as an energy function, where lower energy corresponds to better solutions.
- Mixing Hamiltonian (H_M): Facilitates quantum transitions between different solutions, preventing the algorithm from getting stuck in local minima.

The quantum system evolves through a series of alternating unitary transformations parameterized by angles γ and β . These parameters are optimized using classical algorithms to minimize the cost function.



3. Quantum optimization

Quantum Approximate Optimization Algorithm (QAOA)



3. Quantum optimization

Feedback-based Algorithm for Quantum Optimization (FALQON)

Define a time-dependent Hamiltonian:

$$H(t) = H_c + \beta(t)H_d$$

- H_c is the **cost Hamiltonian**
- H_d is the **driver Hamiltonian**

Update rule of $\beta(t)$:

$$\beta(t) = -A(t) = -i\langle [H_d, H_c] \rangle_t$$

Step 1: Prepare state $|\psi_k\rangle$

Step 2: Measure $A_k = i\langle [H_d, H_c] \rangle_{k\Delta t}$

Step 3: set $\beta_{K+1} = -A_k$

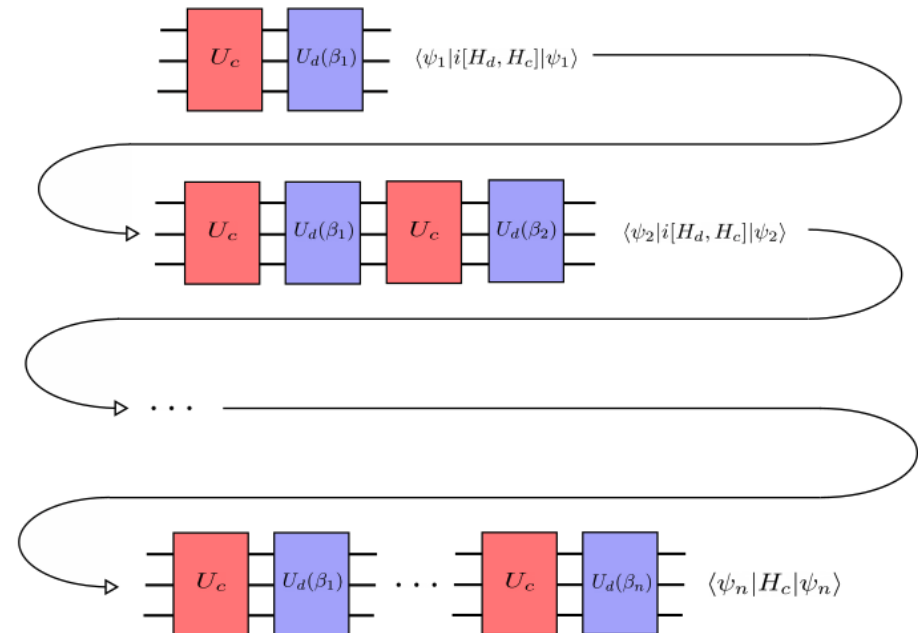


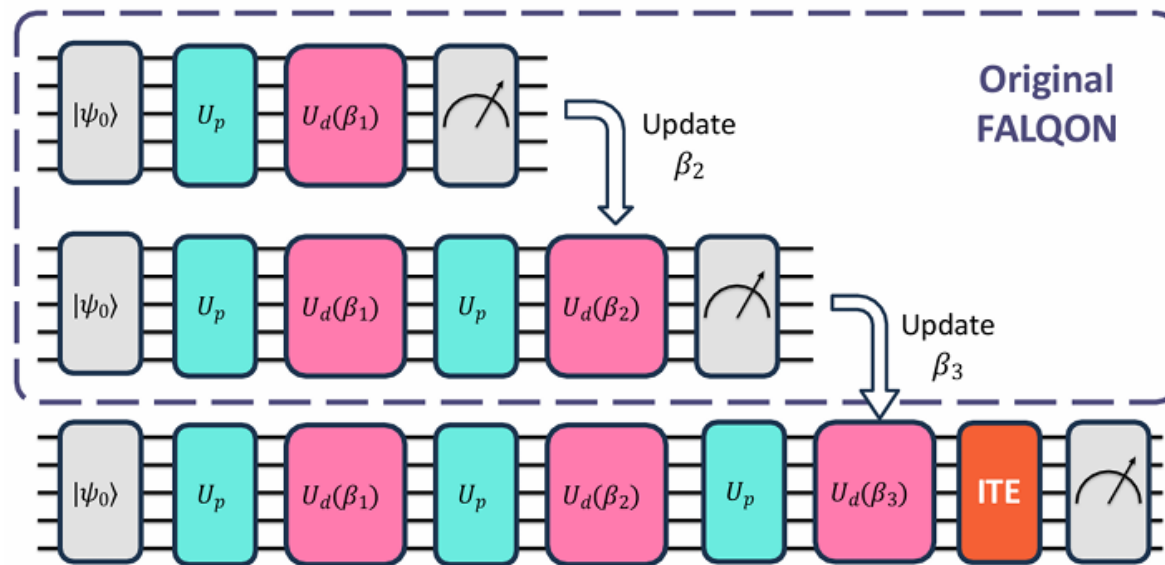
Fig 1. Recursive quantum circuit of FALQON (pennyLane.ai)

3. Quantum optimization

Feedback-based Algorithm for Quantum Optimization (FALQON)

An imaginary time evolution (ITE) is applied every few FALQON steps.

$$|\bar{\psi}\rangle = \frac{(I - \Delta\tau H_p)|\psi\rangle}{\|I - \Delta\tau H_p|\psi\rangle\|}$$



The ITE-FALQON workflow

3. Quantum optimization

FALQON applications: Hubbard model (many-body physics)

A framework used to describe interacting fermions on a lattice.

$$H_{FH} = T + V$$

$$T = -J \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^+ c_{j\sigma} + c_{j\sigma}^+ c_{i\sigma})$$

$$V = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

- i, j : neighboring lattice sites
- σ : spin index ($\uparrow, \downarrow$)
- T : hopping term with amplitude J
- V : on-site interaction with strength U

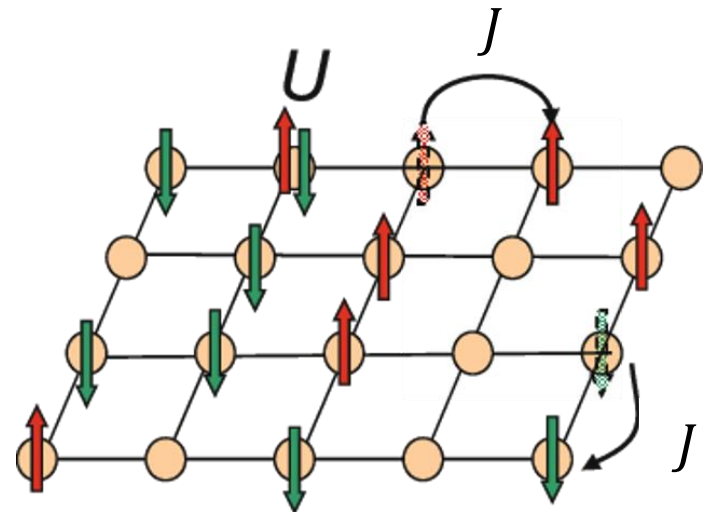
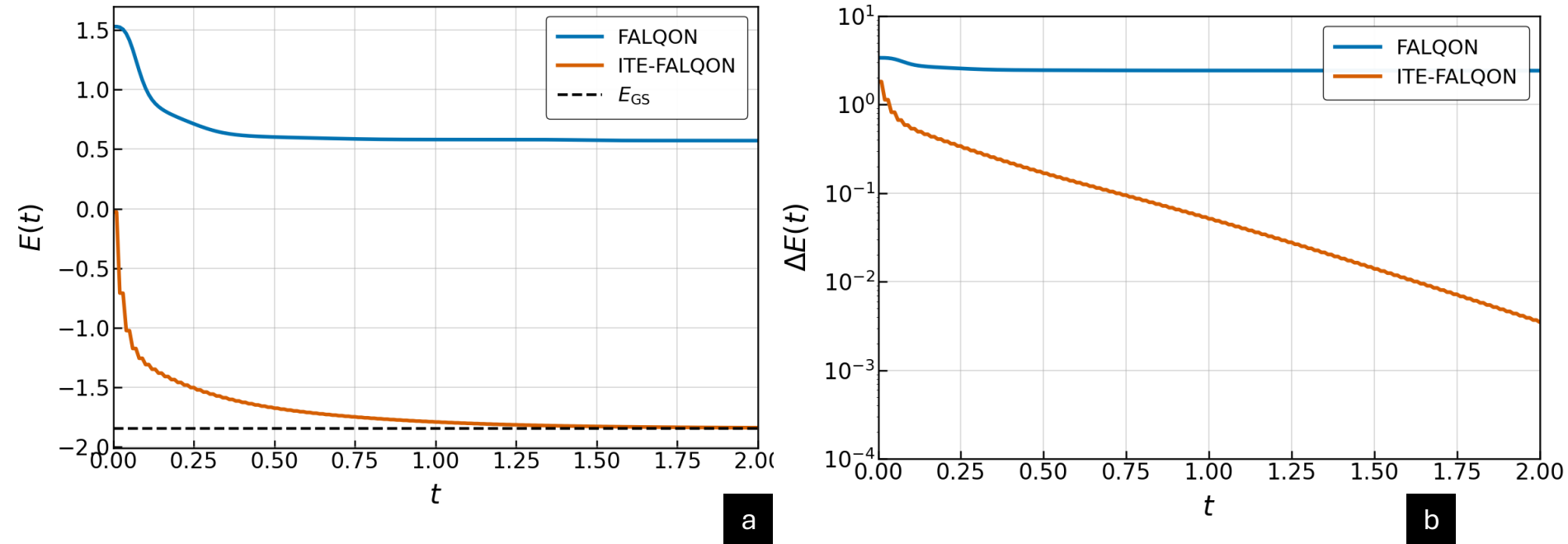


Fig 2. 2D Fermi-Hubbard model
(Susumu Yamada et.al., 2022)

3. Quantum optimization

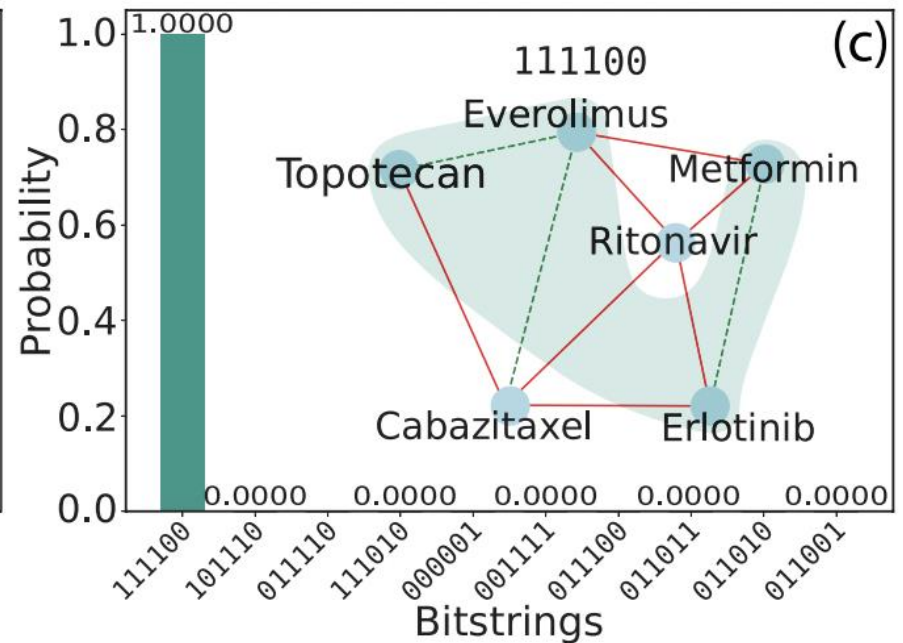
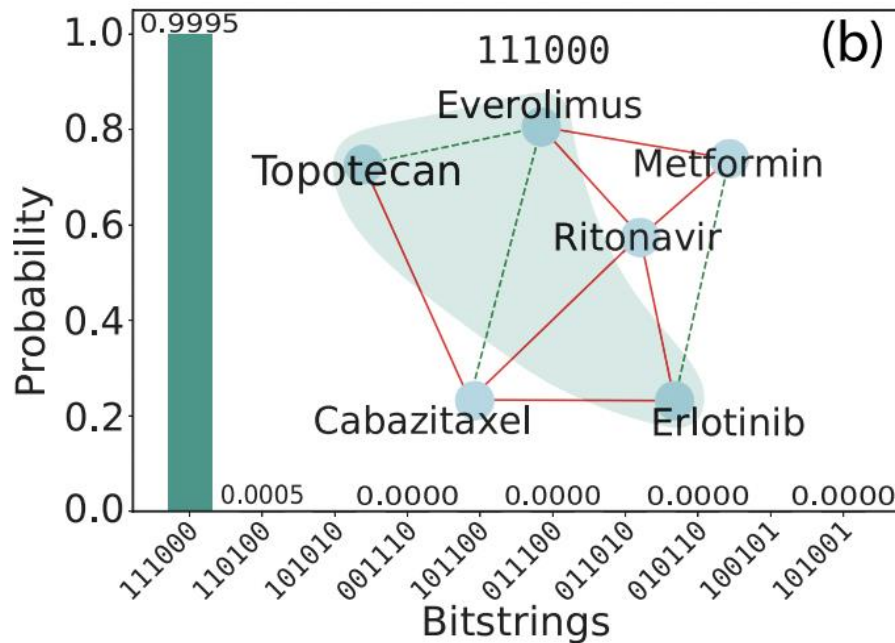
FALQON applications: Hubbard model (many-body physics)



Numerical results for the 2x2 half-filled lattice with and without ITE. (a) Energy evolution of FALQON and ITE-FALQON with ED baseline and (b) is the corresponding energy differences

3. Quantum optimization

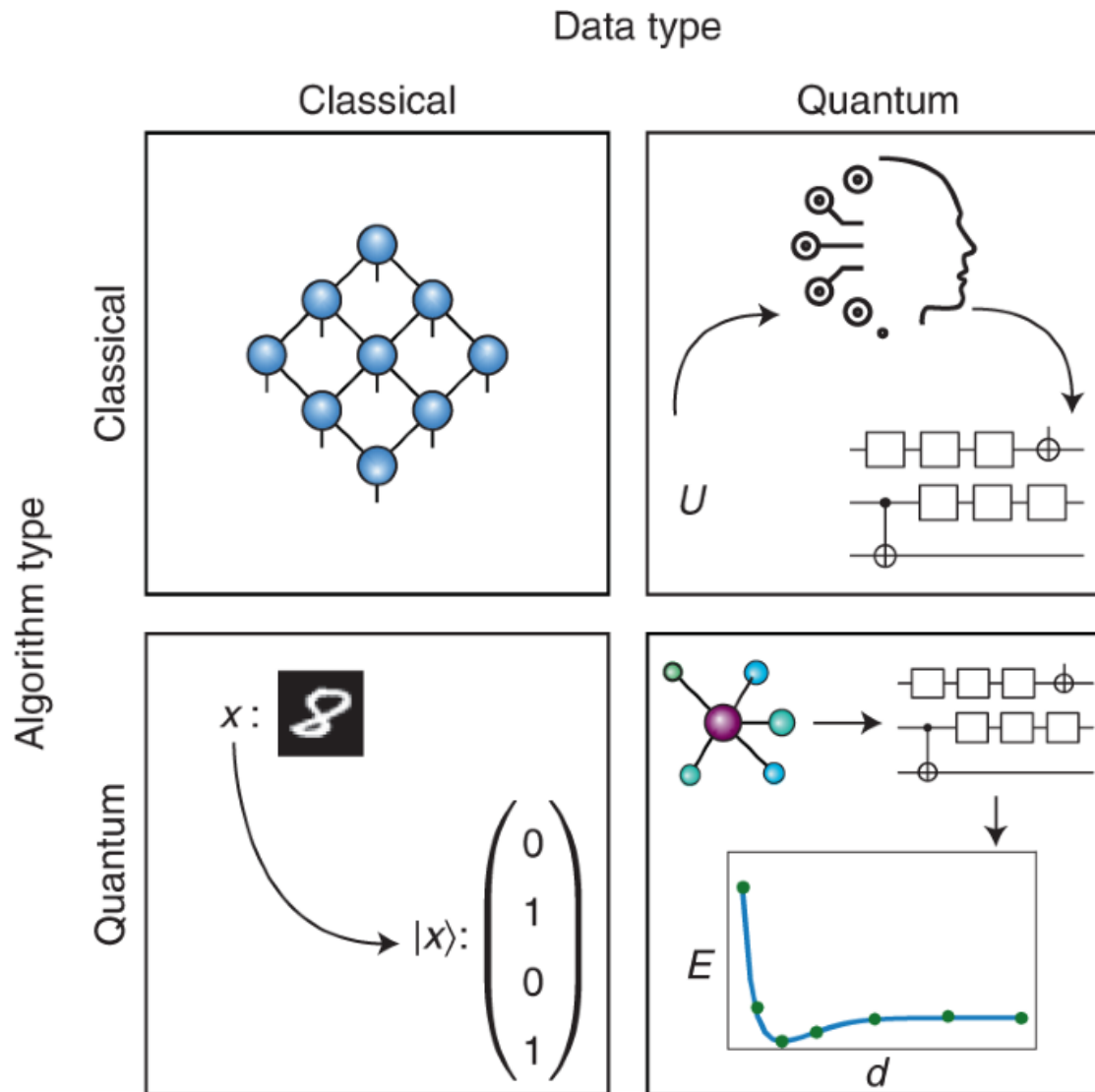
FALQON applications: Drug-drug interaction



Outline

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4. Quantum machine learning



4. Quantum machine learning

QUANTUM ML VS. CLASSICAL ML

ADVANTAGES



- Potential for speedups in high-dimensional problems.
- Naturally handles **quantum data** (e.g., quantum chemistry, material science).
- Can exploit **quantum parallelism** for certain optimization and sampling tasks.



DISADVANTAGES

- **Hardware limitations** (low qubit counts, noise, short coherence times).
- **Data encoding bottleneck** — often nullifies theoretical speedups for classical data.
- Algorithms may give only *polynomial* speedups, not always exponential.
- Still an **active research area**; few real-world advantages demonstrated yet.

4. Quantum machine learning

Developing frameworks and new algorithms

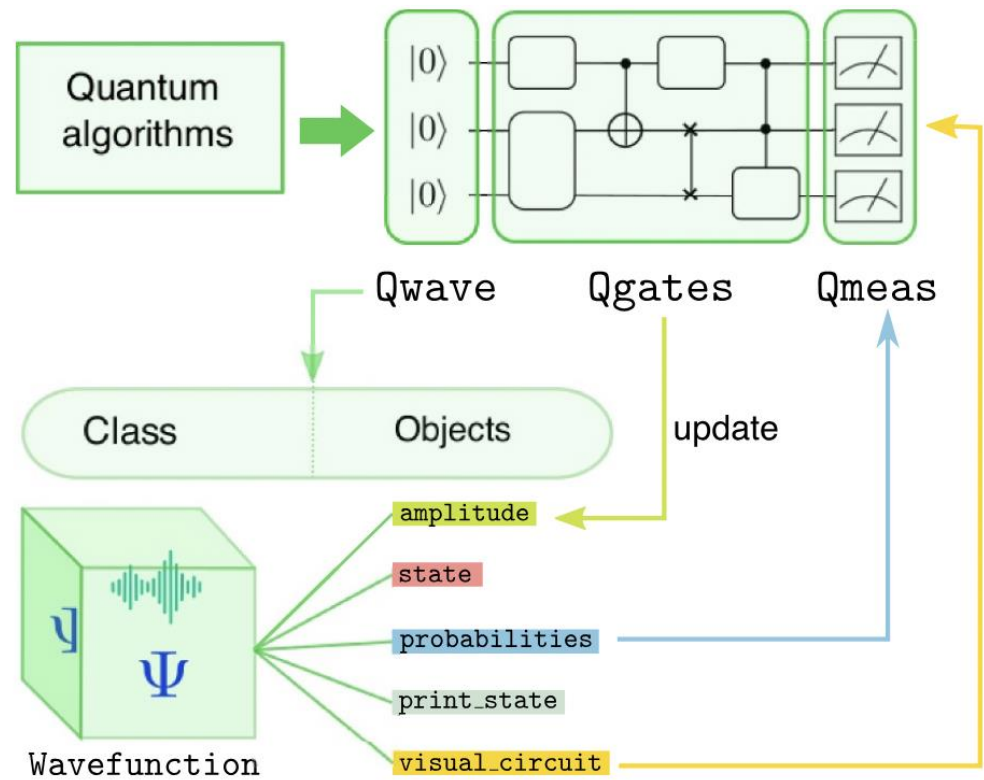
2022, in the collaboration with scientists from HUS-VNU, we developed **QSun**, a framework for QML



Prof. Le Bin Ho,
Tohoku University



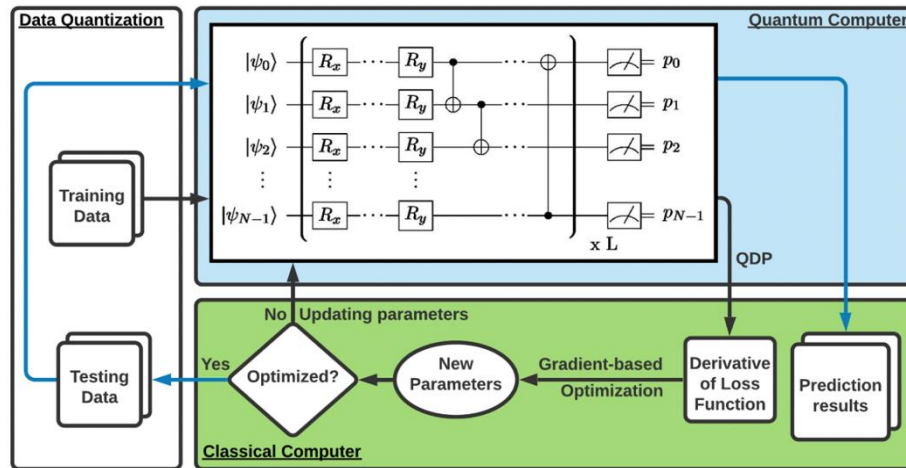
N. Q. Chuong,
(Duy Tan University)



C. Q. Nguyen et al. *Mach. Learn.: Sci. Technol.* **3** (2022) 015034

4. Quantum machine learning

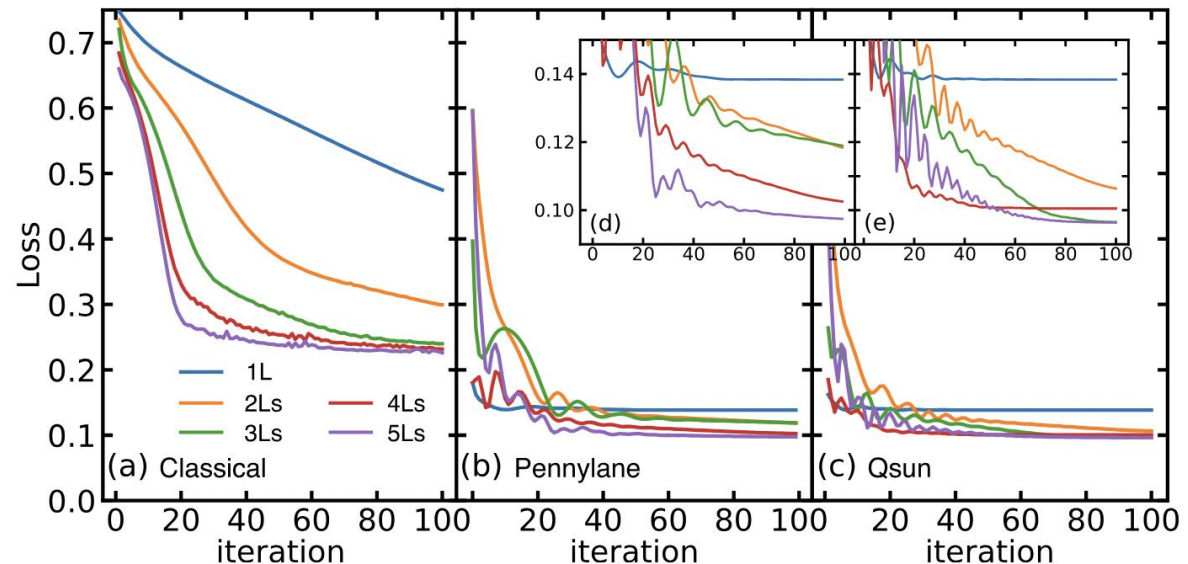
Developing frameworks and new algorithms



Quantum neural network (QNN) in hybrid quantum-classical framework



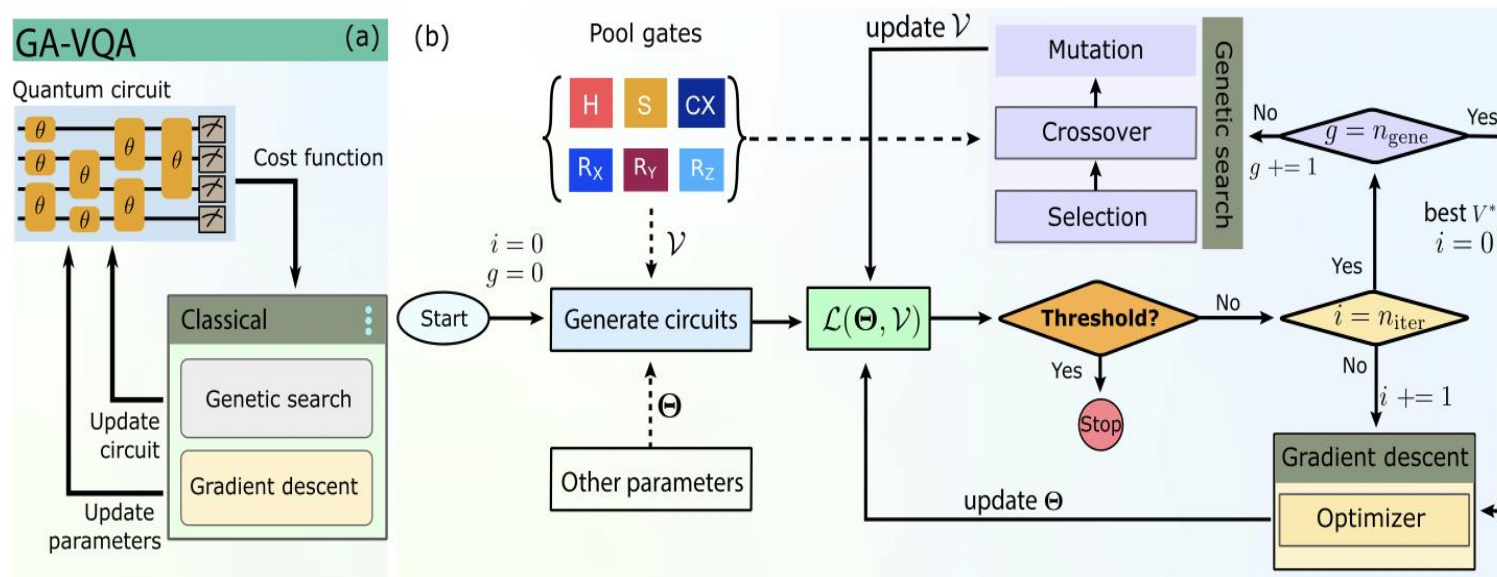
N. Q. Chuong,
(Duy Tan University)



4. Quantum machine learning

Developing frameworks and new algorithms

2024, we developed GA-VQA framework for quantum circuit generation



Vu Tuan Hai, PhD
Student
Nara Institute of Science
and Technology

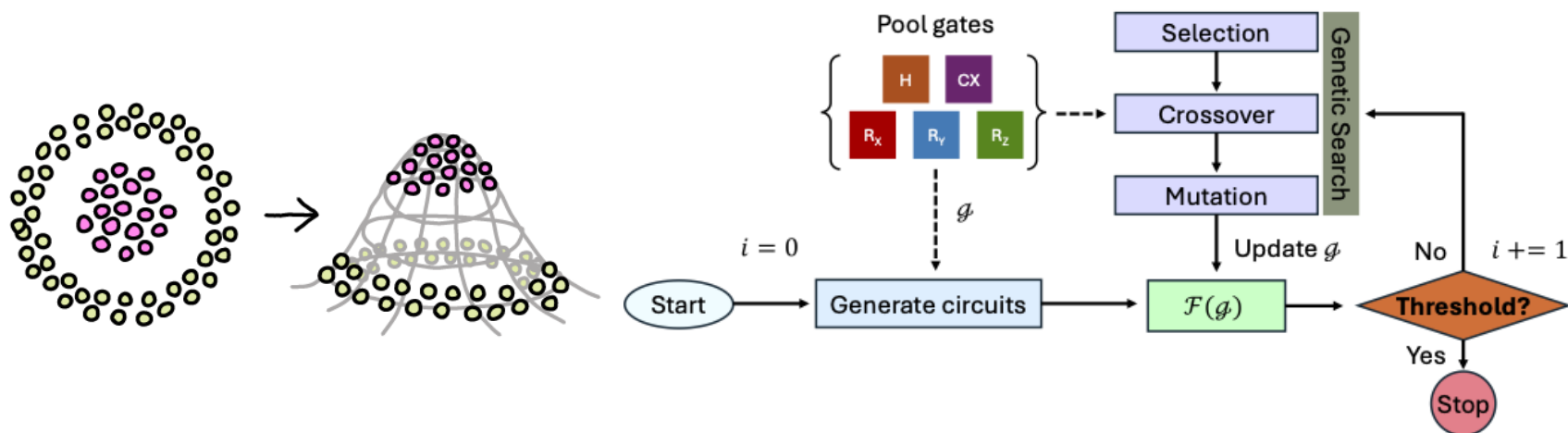


Prof. Le Bin Ho,
Tohoku University

4. Quantum machine learning

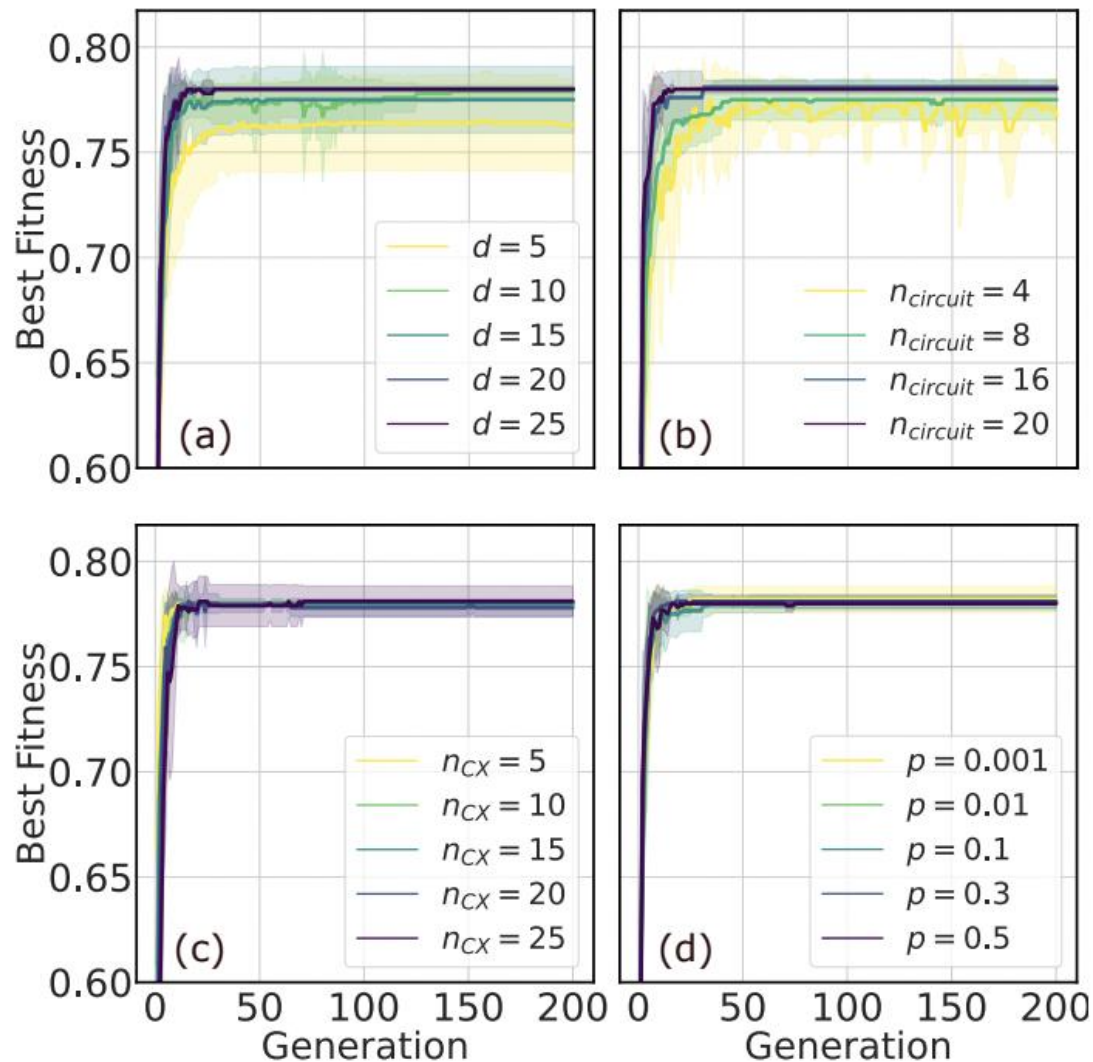
Developing frameworks and new algorithms

- We are currently working on quantum support vector machine (QSVM) using GA-VQA
- QSVM is important for **virtual screening**



Model	Feature maps	Num qubits (PCA)		
		3	4	5
Classical SVM	RBF	0.9666	0.9706	0.9706
Quantum SVM	RX and CNOT	0.9615	0.9615	0.9692
	Genetic Algorithm	0.9607	0.9719	0.9831

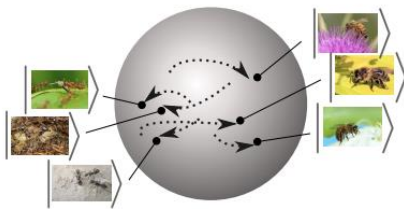
4. Quantum machine learning



4. Quantum machine learning

Currently, we are developing trainable kernel QSVM (TK-QSVM)

a. Training the embedding



b. Classification

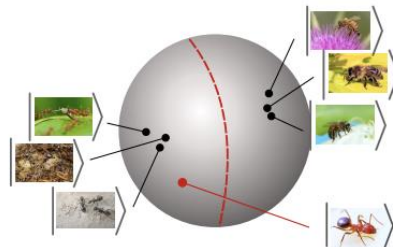


FIG. 1. Illustration of quantum metric learning. a. The embedding is trained to maximize the distance of the data clusters in the Hilbert space of quantum states. b. The measurement used to classify new inputs depends on the distance measure used. The simple decision boundary in Hilbert space can correspond to a highly complex decision boundary in the original data space.

Seth Lloyd et al. [arXiv:2001.03622](https://arxiv.org/abs/2001.03622)

Inner-product loss:

$$L_i(\theta) = 1 - \frac{1}{L} \sum_{j=1}^L \frac{1}{M_j} \sum_{i=1}^{M_j} \left| \langle \psi(x_i^j, \theta), y_j \rangle \right|^2$$

Trace-distance loss:

$$L_d(\theta) = 1 - D_{tr}(\rho_A, \rho_B)$$

with $D_{tr}(\rho_A, \rho_B) = \frac{1}{2} \text{Tr} |\rho_A - \rho_B|_1$

Maximize Likelihood loss:

$$\begin{aligned} L_{mle}(\theta) &= -\log \left(\prod_{j=1}^L \prod_{i=1}^{M_j} \left| \langle \psi(x_i^j, \theta), y_j \rangle \right|^2 \right) \\ &= -\sum_{j=1}^L \sum_{i=1}^{M_j} \log \left(\left| \langle \psi(x_i^j, \theta), y_j \rangle \right|^2 \right) \end{aligned}$$

ND Quyen, **TNL**, and others [arXiv:2607.12487](https://arxiv.org/abs/2607.12487)

4. Quantum machine learning

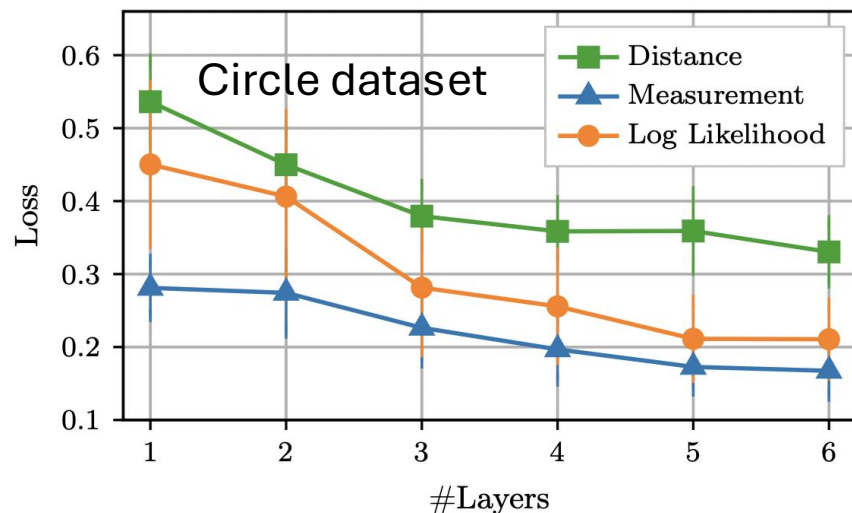
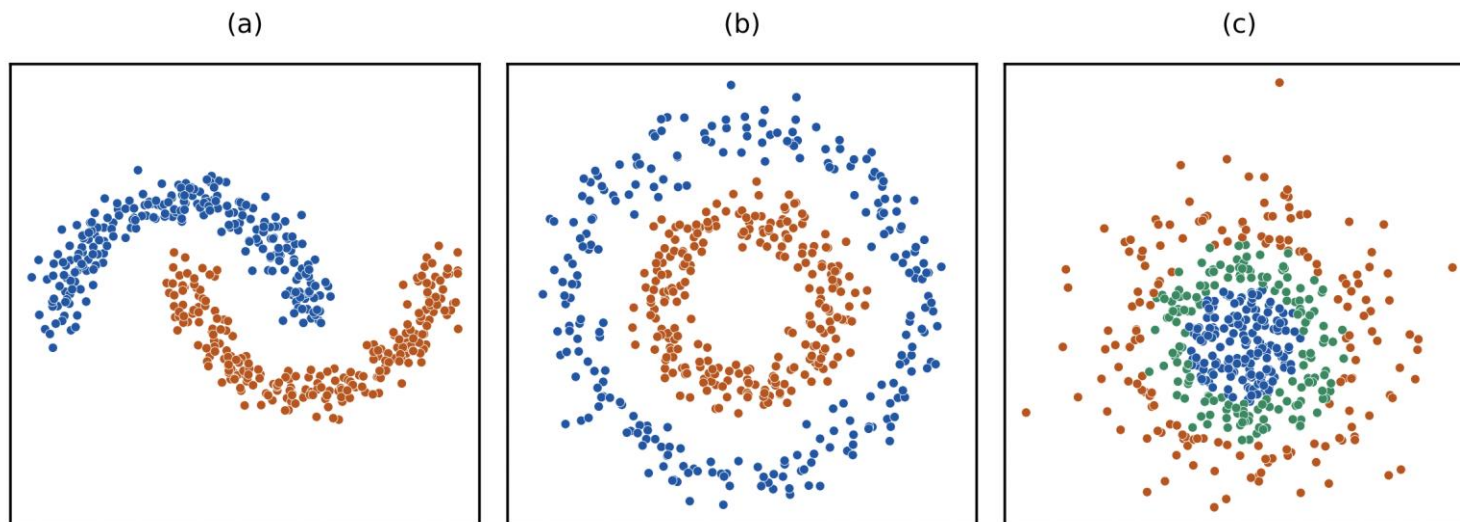


TABLE IV. Test accuracy of the LLL method with $\#Layers = 4$, with and without simulated noise (depolarizing 0.001/0.01 for one-/two-qubit gates, readout error 0.01, 1024 shots), reported as mean $\pm$ standard deviation over 20 runs.

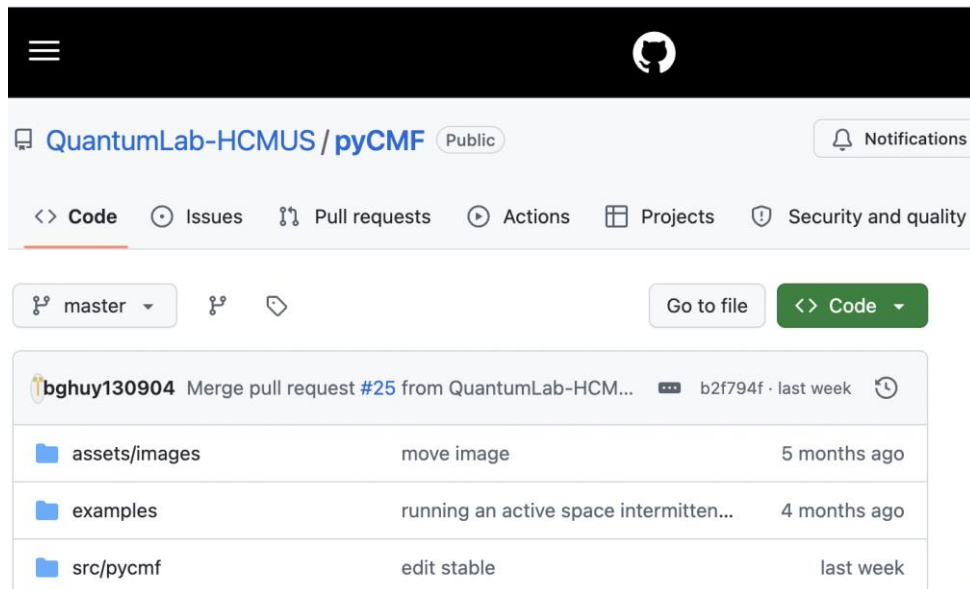
Dataset	Noise-free	With noise
moons	0.97 ± 0.02	0.98 ± 0.02
circles	0.97 ± 0.03	0.91 ± 0.07
gaussian	0.94 ± 0.02	0.85 ± 0.03

5. Summary

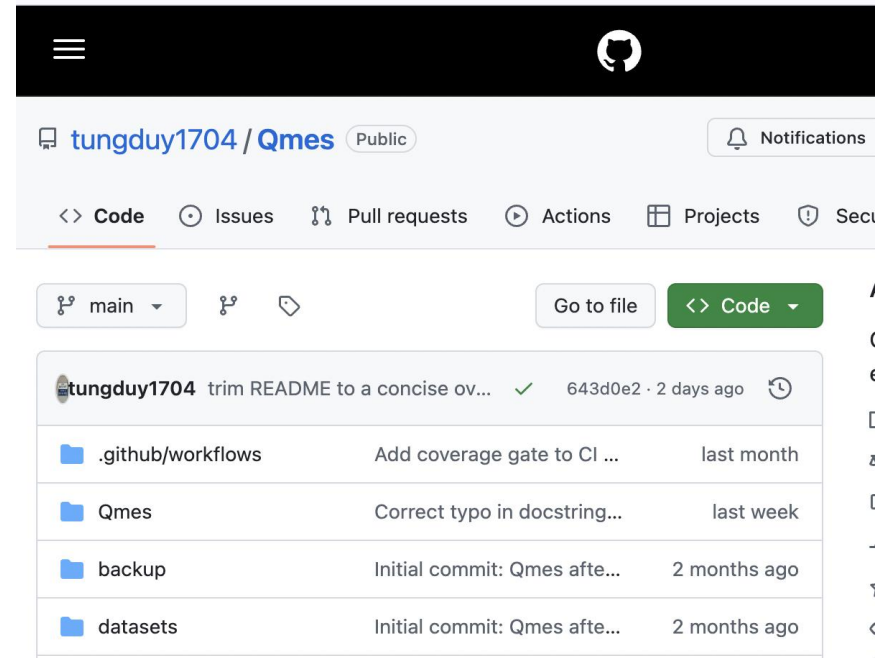
- Quantum computing, in principle, can be used for any steps in drug design strategy
- We are currently focusing on:
 - Developing new framework and algorithms quantum molecular simulation.
 - Developing quantum optimization methods for QUBO problems.
 - Developing QML methods for virtual screening and data analyses.
- We have obtained some proof-of-concepts results → **“realistic” simulation**

Recent news in Quantum at VNUHCM

1. BSc. Program on Quantum Technology (VNUHCM-US, launched in 2027)
2. MSc. Program on Quantum Technology (VNUHCM-US, in preparation)
3. HPC Lab for Quantum Computing (VNUHCM, launched in 2027)
4. Center of Excellence in Quantum Technology (VNUHCM – under preparation)
5. Laboratory for Quantum Technology (VNUHCM - under preparation)



pyCMF: quantum molecular simulation



Qmes: quantum machine learning



Thank you very much for your attention!



Visit us at quantumlab.vn