Introduction to Quantum Computing

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Outlines

1. Quantum Advantage
2. Fault-tolerant quantum computer
3. NISQ
4. Quantum software

1 Quantum Advantage

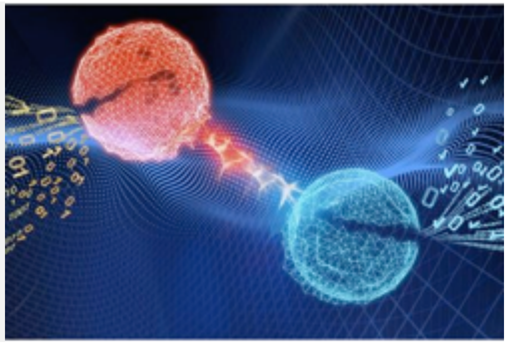
Quantum Technology Overview

Quantum Computing

1. factoring
2. searching
3. optimization
4. scientific computing
5. machine learning

Quantum Simulation

1. high Tc
2. new materials
3. chemical reaction
4. drug discovery
5. novel states

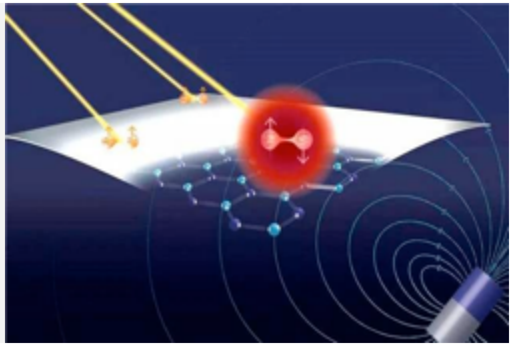


Quantum Communication

1. quantum internet
2. key distribution
3. teleportation
4. encryption
5. direct communication

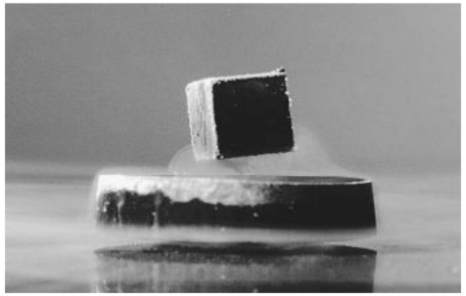
Quantum Sensing

1. gravity
2. magnetic
3. atomic clock
4. GPS



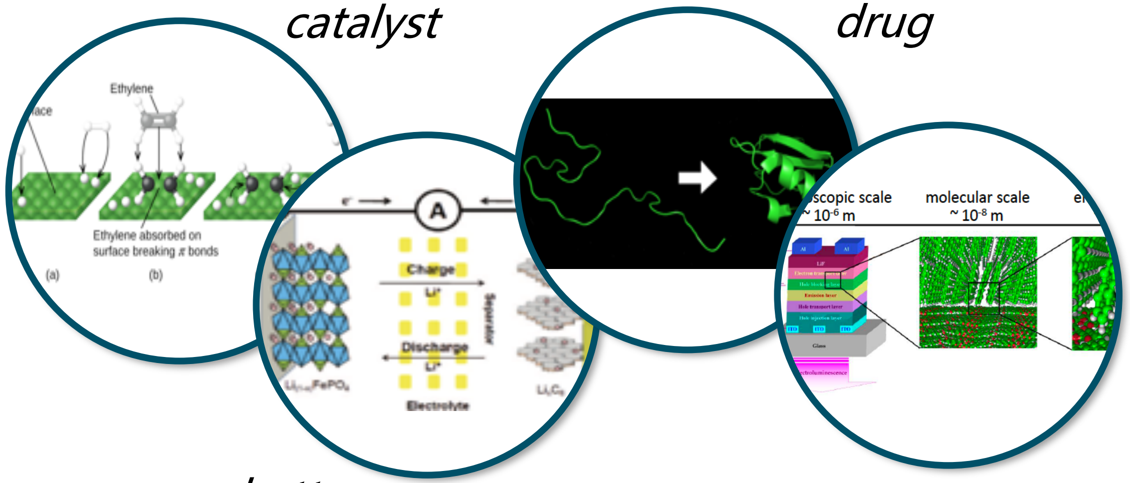
Case Study 1: Quantum Simulations

Simulations of quantum systems (i.e. quantum simulations) are important in advancing our knowledge in many frontiers:



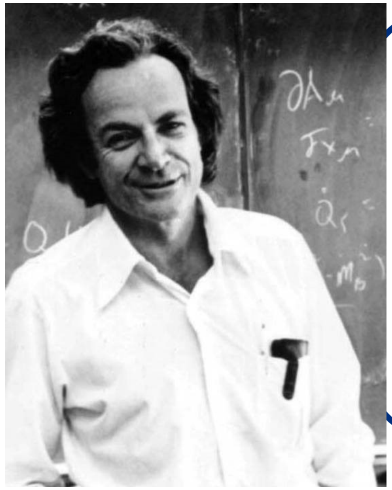
Discovery of high-temperature superconductor

catalyst *drug*



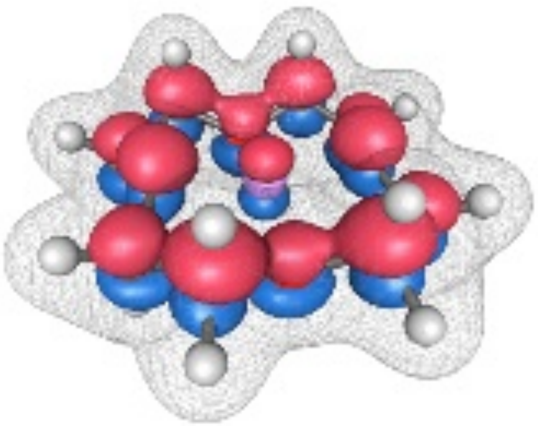
battery *material*

Simulating these many-body quantum systems with classical computers is difficult due to the exponential scaling.



Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical

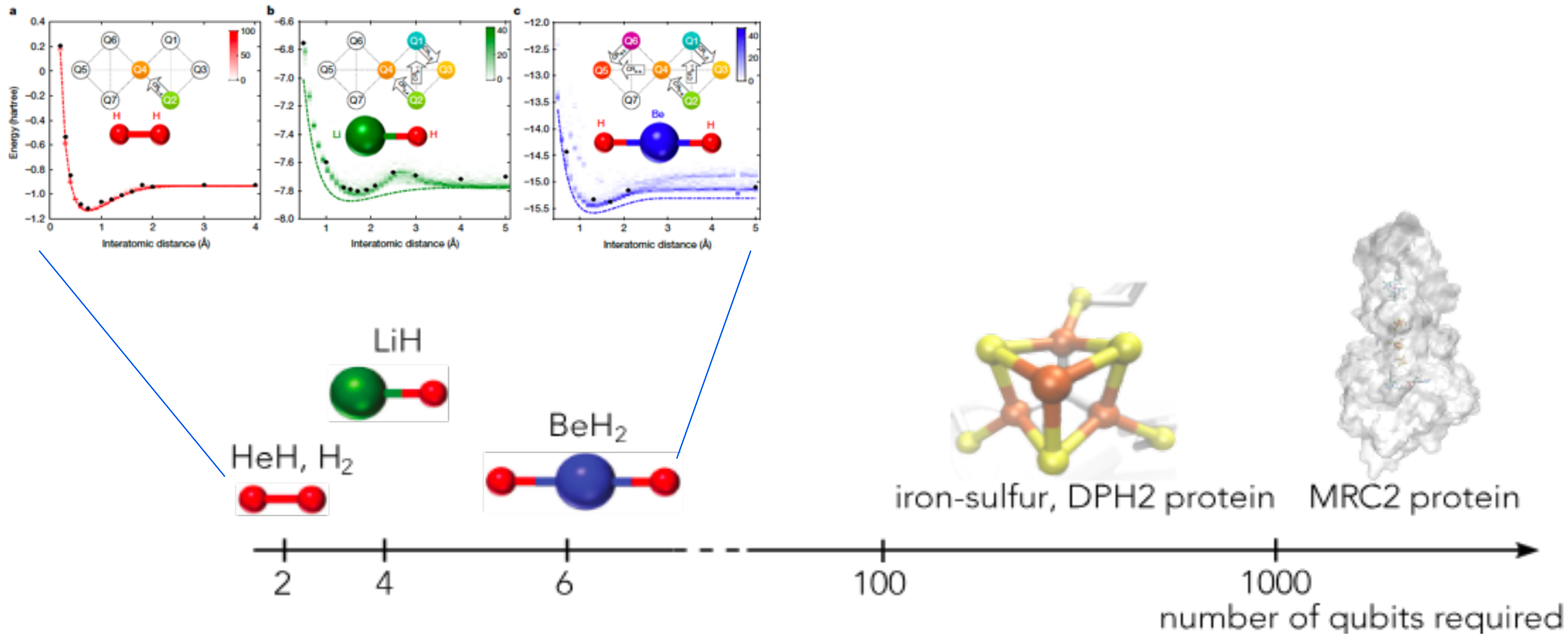
Case Study 1: Quantum Simulations



Each qubit encodes one atom orbital

number of orbitals	memory
10	16 kByte
20	16 MByte
30	16 GByte
40	16 TByte
50	16 EByte
60	16 ZByte
…	…
250	all atom in the universe

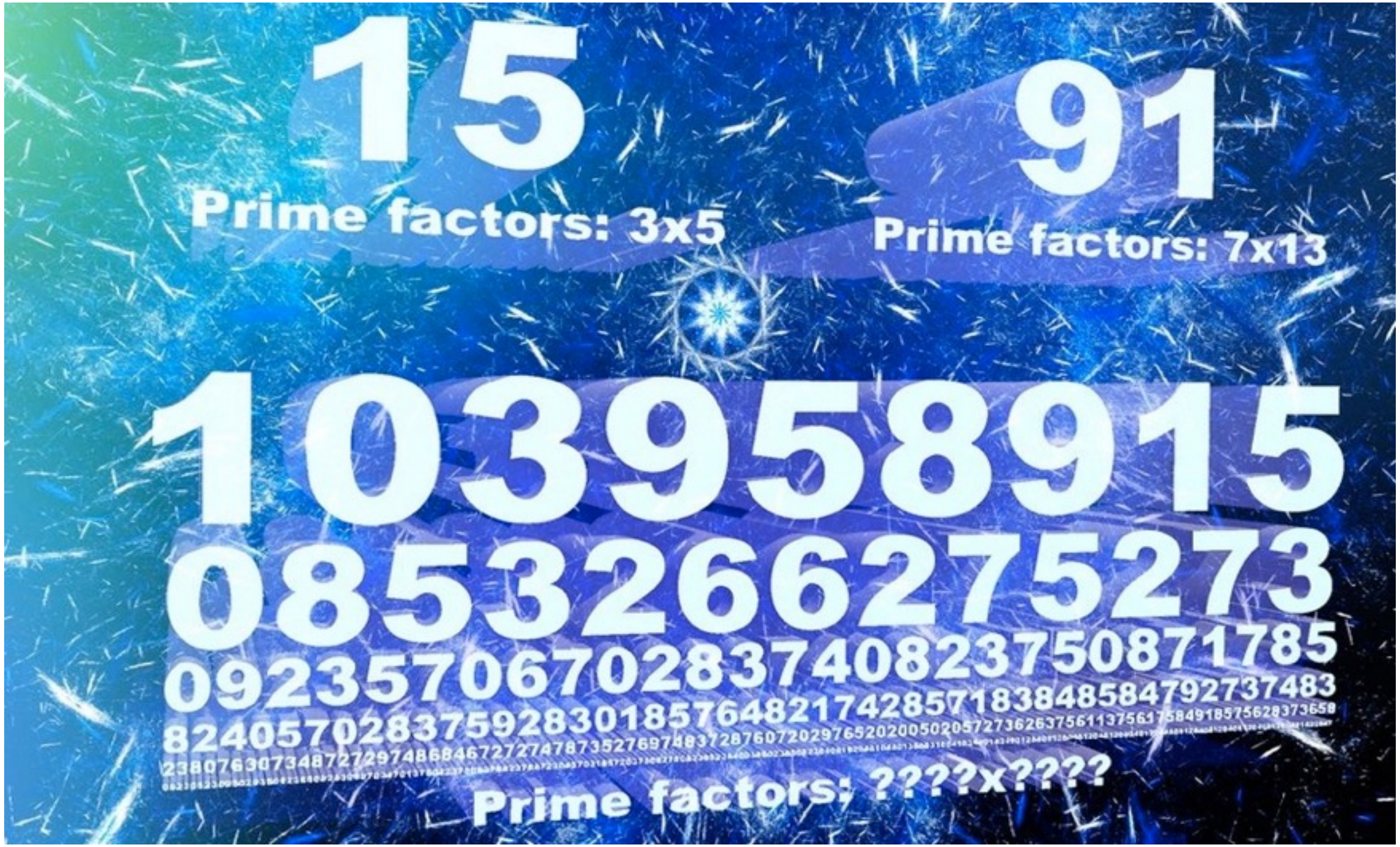
Case Study 1: Quantum Simulations



Classical computing fails very soon with
the size of molecules increase

Case Study 2: Factoring

Shor Algorithm: break down the modern cryptography infrastructure

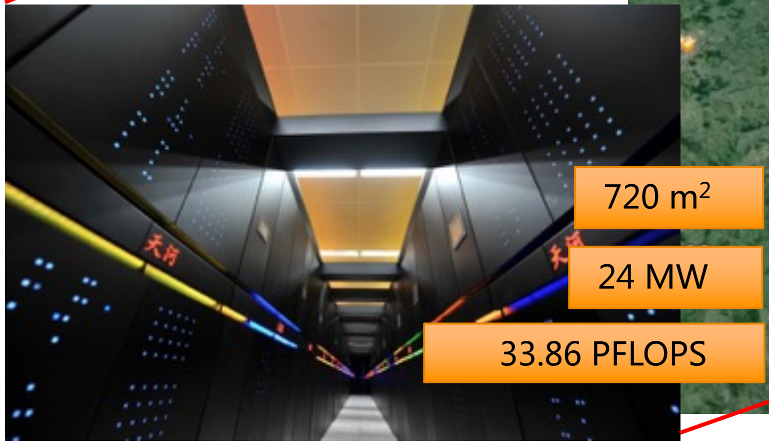


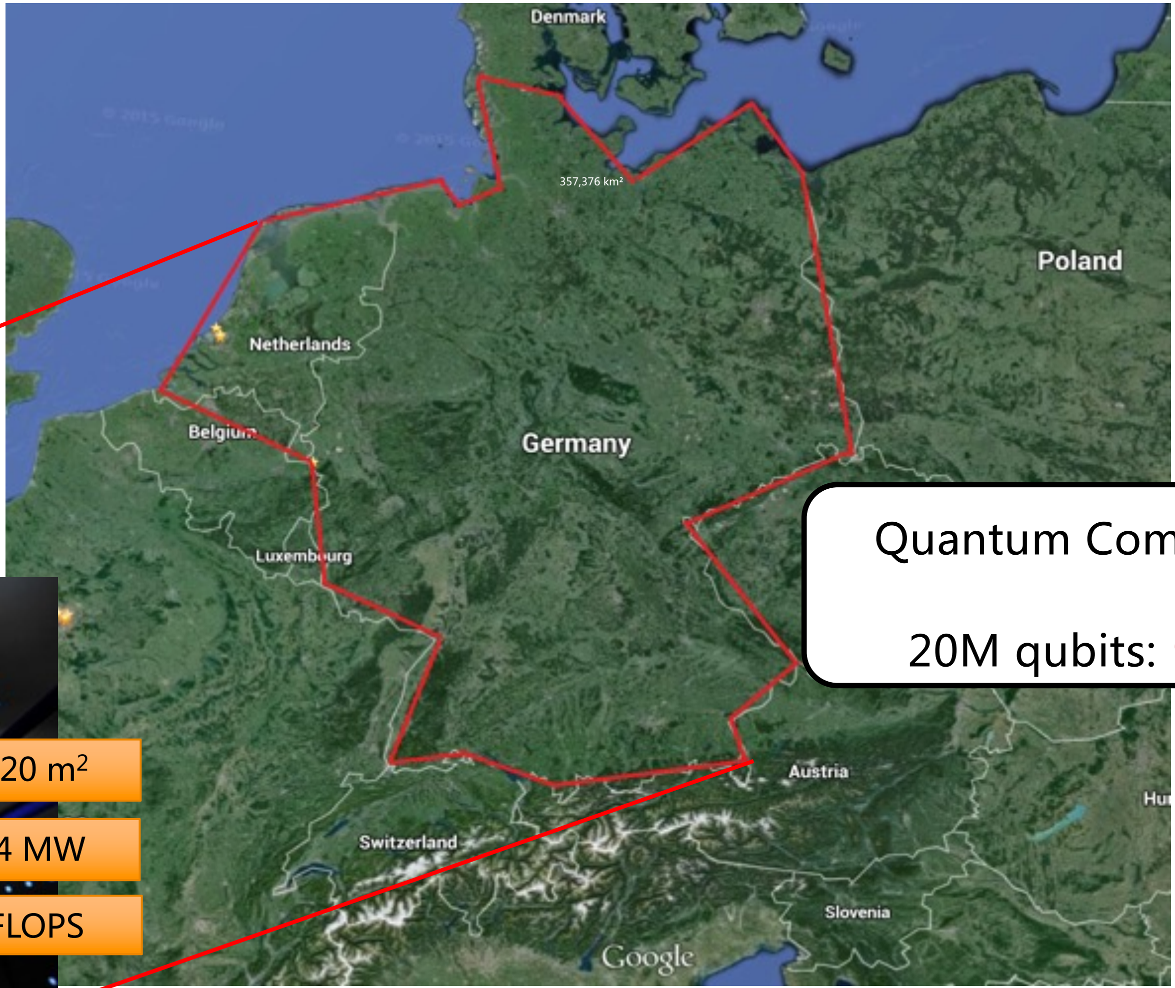
Case Study 2: Factoring

Problem: factor
2048bits number

Classical Approach

~ **100** y
~ 10^{18} RMB
~ 10^{19} Watt





Quantum Computer with
20M qubits: **8** hours

Exponential Acceleration!

Adapted from J. Martinis Slides

Case Study 3: Searching

Grover algorithm: Unsorted database search

Have to try $N/2$ keys on average

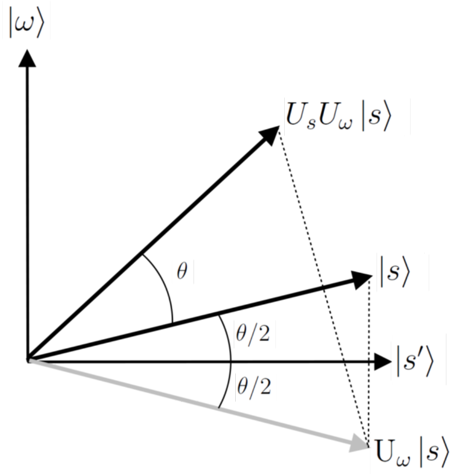
Classical approach

N keys

For one lock

Quadratic Acceleration in Query!

Only requires $\sqrt{N}$ trials



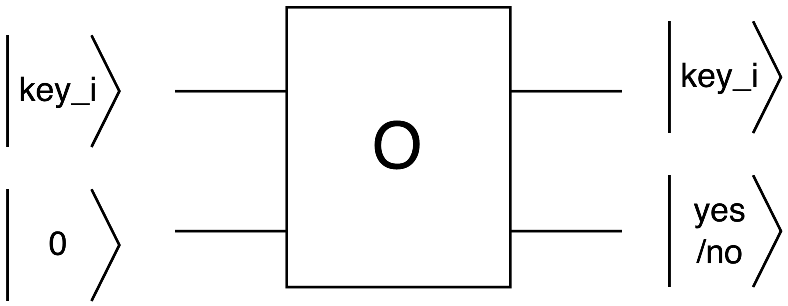
Grover search

Quantum approach

Case Study 3: Searching

Disclaimer

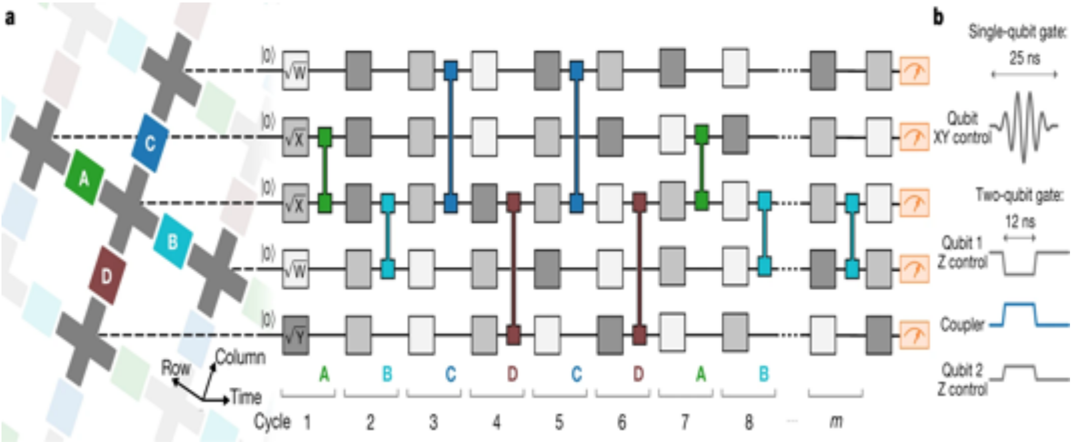
- Structured database (binary tree) has efficient classical searching algorithm: $\ln N$
- The quadratic acceleration is also the upper bound,
  we cannot do better using quantum (implying quantum also fails NPC)
- The quantum oracle - what is a key trial in quantum sense ?
  Are we comparing apple to orange?



$$O(\sum_i |i\rangle|0\rangle) = \sum_i |i\rangle|o(i)\rangle$$

Make use of the superposition
nature of quantum mechanics

Case Study 4: Quantum Supremacy



All three cases before are in theory and require fault-tolerant quantum computer to run, the supremacy case study is instead feasible on current noisy hardware

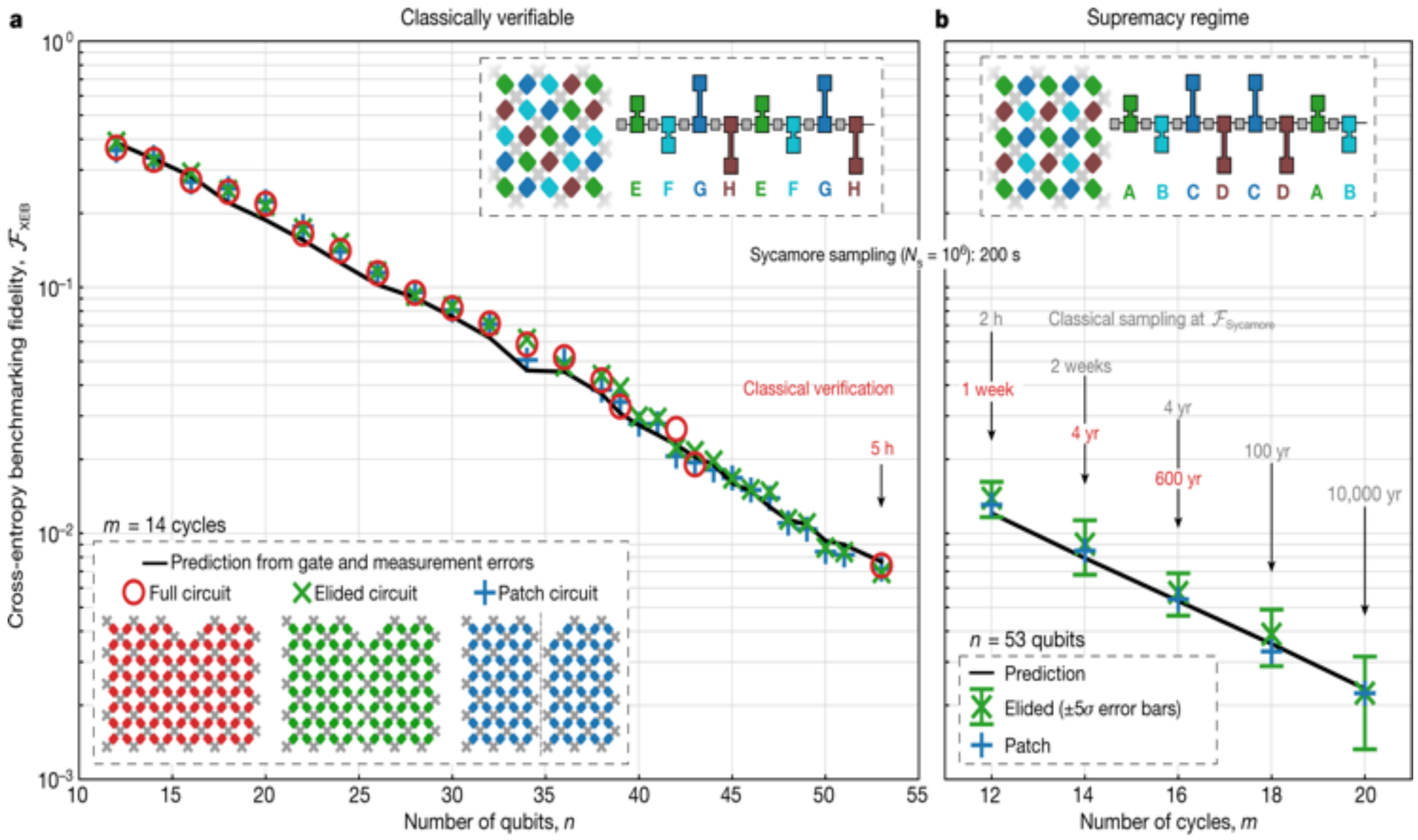
Superconducting:

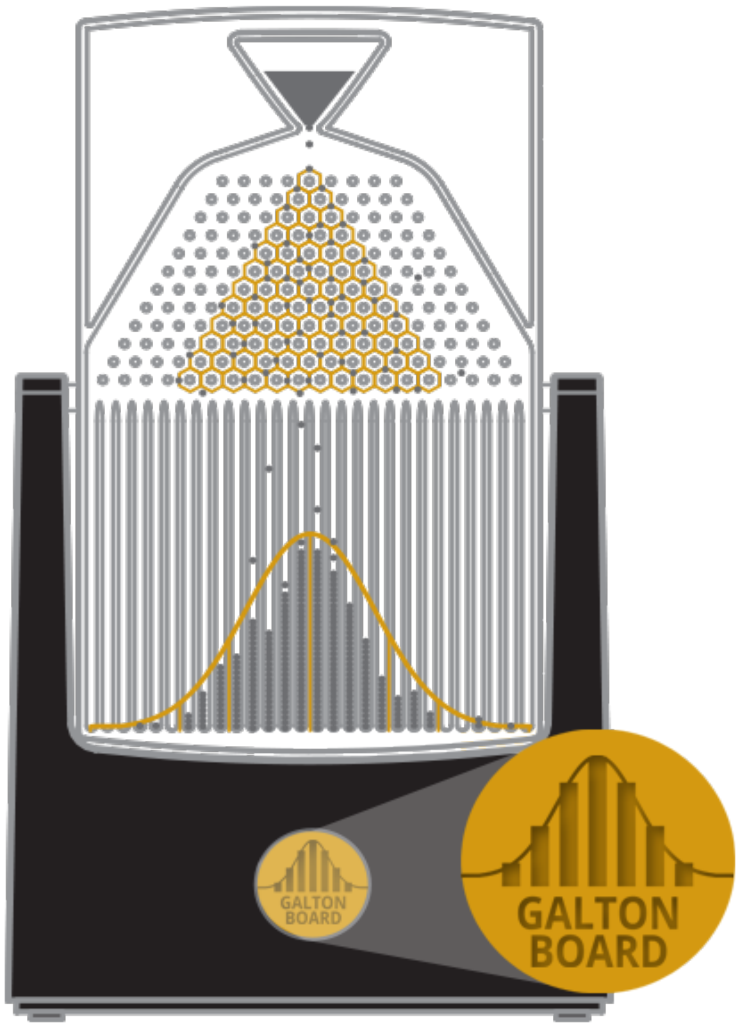
2019 Google Sycamore 2024
2021 USTC Zuchongzhi 2024

Photonic:

2020 USTC Jiuzhang
2022 Xandau Borealis

Case Study 4: Quantum Supremacy





A probability sampling task

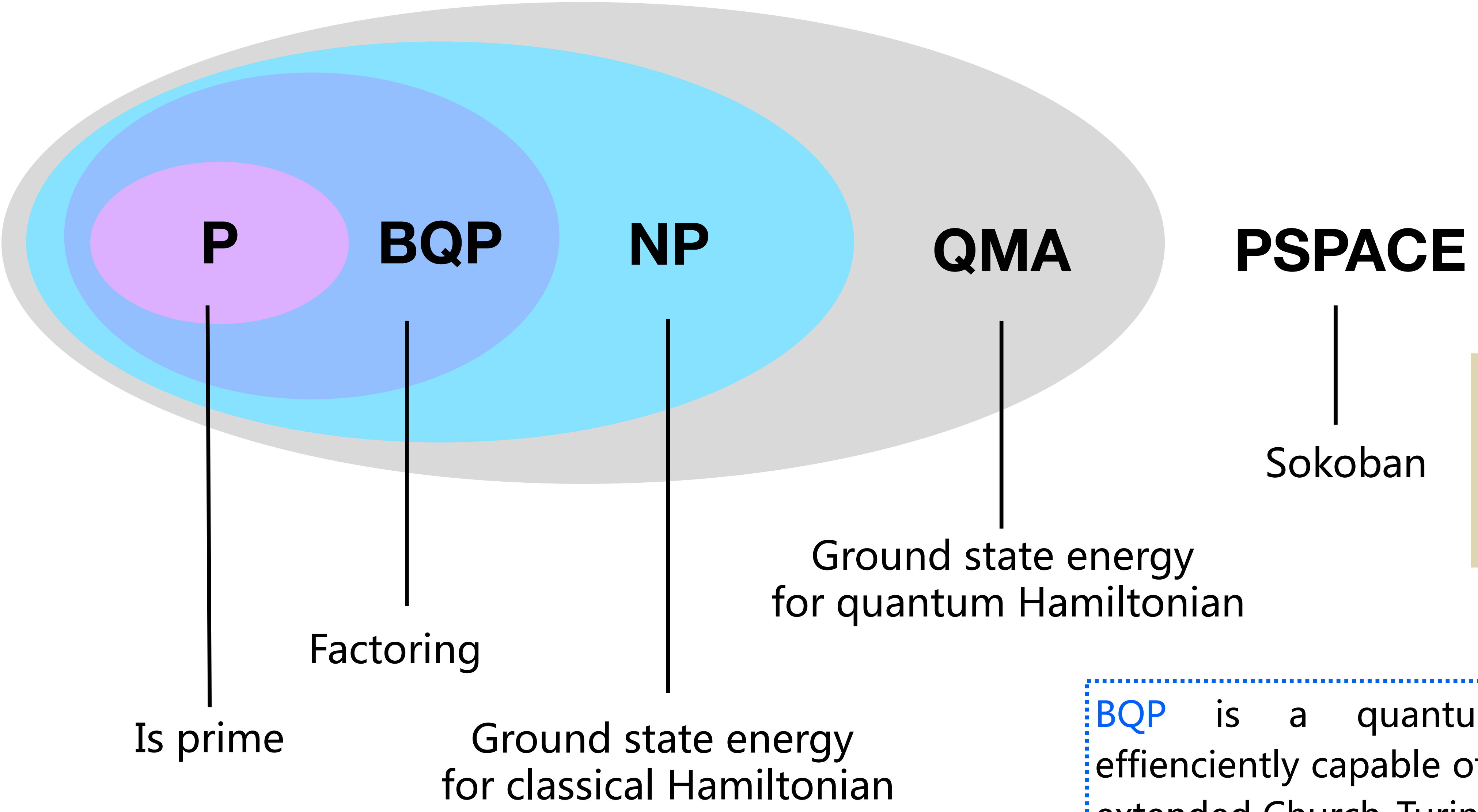
Case Study 4: Quantum Supremacy

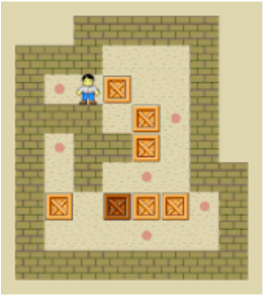
Disclaimer

- The task is of no practical use
- Expected xeb result: 1 = quantum behavior; 0 = classical behavior;
  Experimental result: < 0.01
- XEB estimation itself requires the classical simulation of the circuit amplitude
- The initial claim by Google - thousands of years classical computing estimation is outdated. Current tensor network based simulation approach can fully close the gap and outperform Google’s 2019 experiments even in running time.

arXiv:2005.02421
PRL.129.090502
arXiv:2406.18889

Summary: Quantum Complexity





BQP is a quantum computer effiencientl capable of: breaking the extended Church-Turing thesis

2

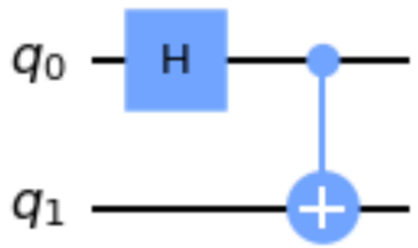
Fault-Tolerant Quantum Computer

Quantum Computing: Brief History

- Benioff, 1980
  Quantum Turing machine
- Feynman, 1981
  Simulate quantum with quantum
- Deutsch, 1985
  Universal quantum computer

- Shor, 1994
  Shor Algorithm for factoring
- Grover, 1996
  Grover Algorithm for searching
- Lloyd, 1996
  Universal quantum simulators

- *Circuit Model*



$$CX \; H \otimes I \; |0\rangle \otimes |0\rangle$$

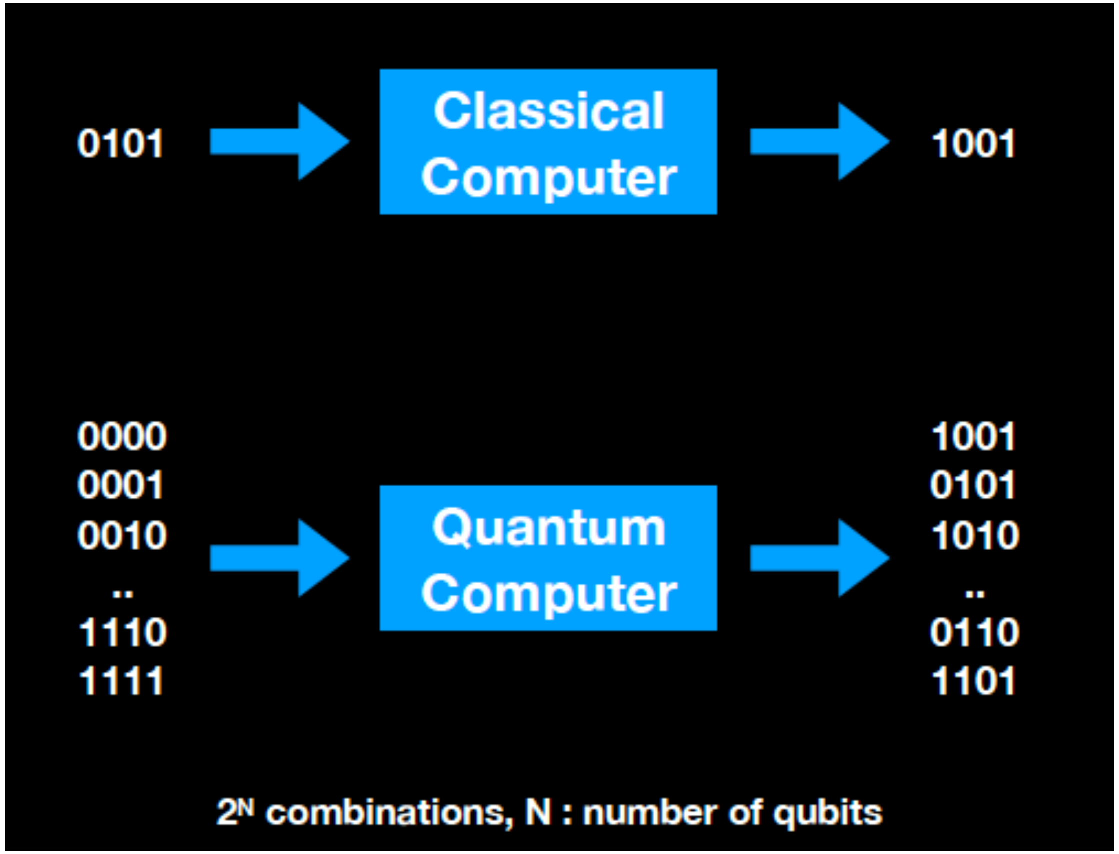
$$\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & & 1 \\ & & 1 & \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & & \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & & \\ & & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ & & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix}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

Quantum Computing: Brief History

- Question: is there any practical application that quantum computer provides advantage?
- Answer by Shor: Prime Factorization (1995)
- Further established by quantum complexity theory:
  P <(?) BQP <(?) NPC
  Quantum computation is useful!

- Question: inevitable quantum noise will destroy any meaningful output
- Answer by Shor: Shor code for error correction (1995)
- Further established by fault tolerant quantum computation theory: noise free quantum computer is possible as long as the physical infidelity is lower than some threholds
  Quantum computation is feasible!

Quantum Computing in a Nutshell

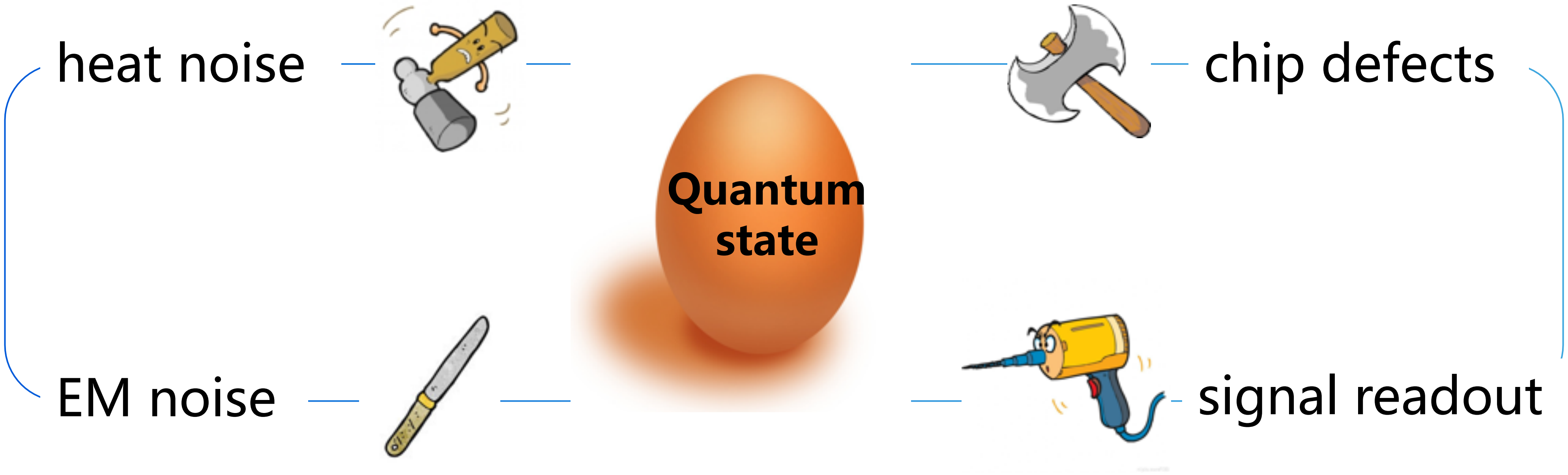


Superposition+entanglement enable us the exponential parallel computing capability, but measurement restricts us from efficiently extracting the information.

The quantum advantage is highly **nontrivial**. The correct way for inference is the key.

superposition + entanglement + measurement

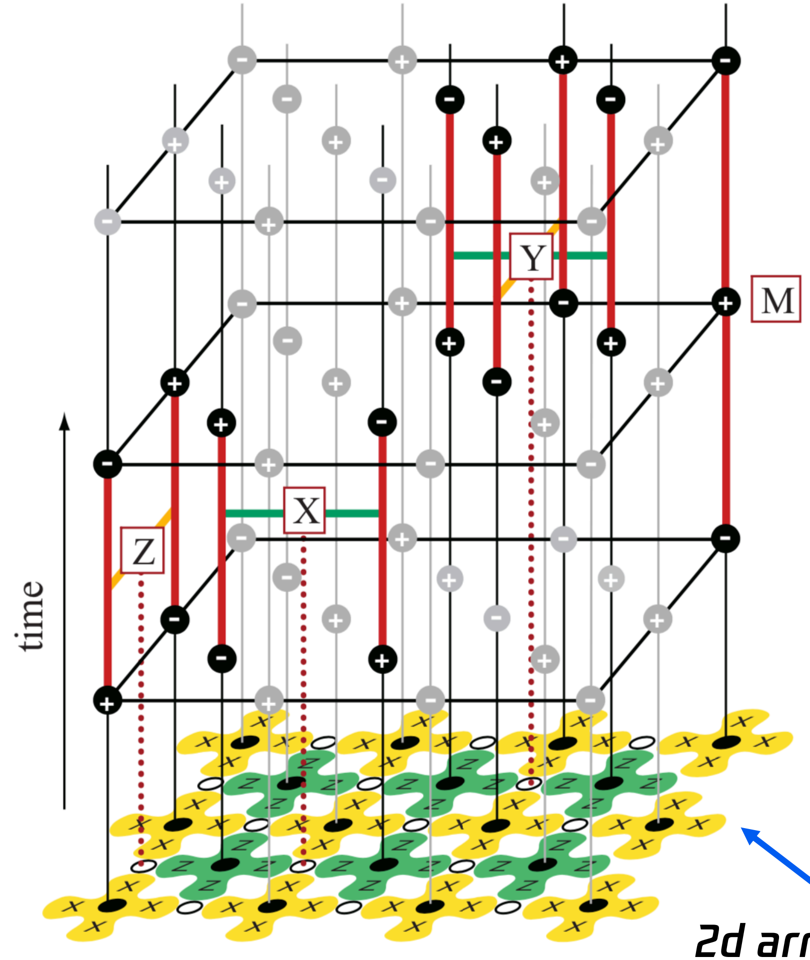
Quantum Computing: Decoherence



Fault tolerant quantum computing is feasible with small infidelity, but require tremendous qubit overhead

Quantum Computing: Error correction code

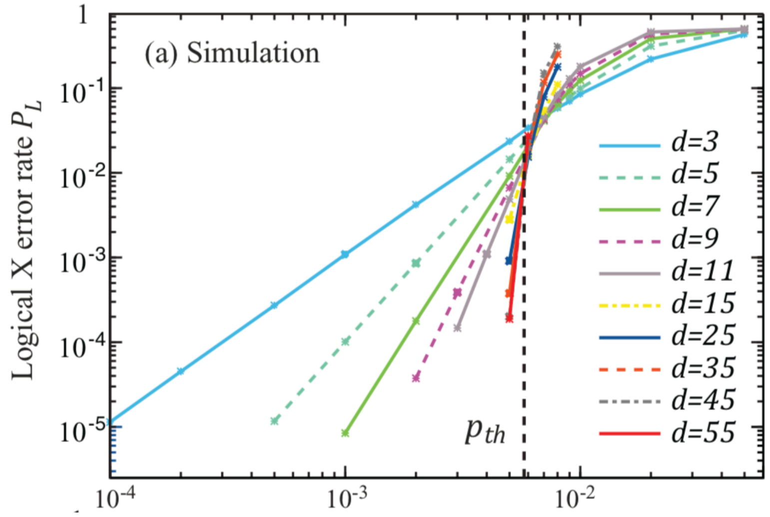
- **Surface code**



2d array physical qubits

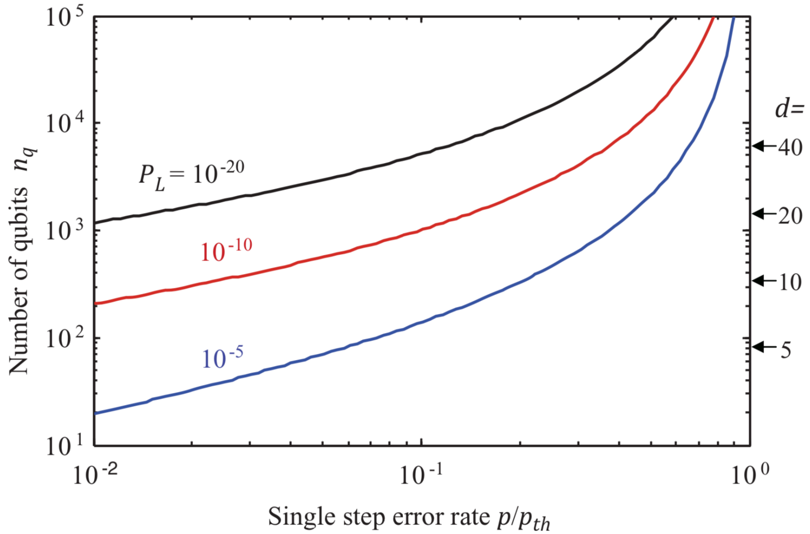
- **Threshold theorem**

PhysRevA.86.032324



Fidelity sota now is below threshold

Google 2024



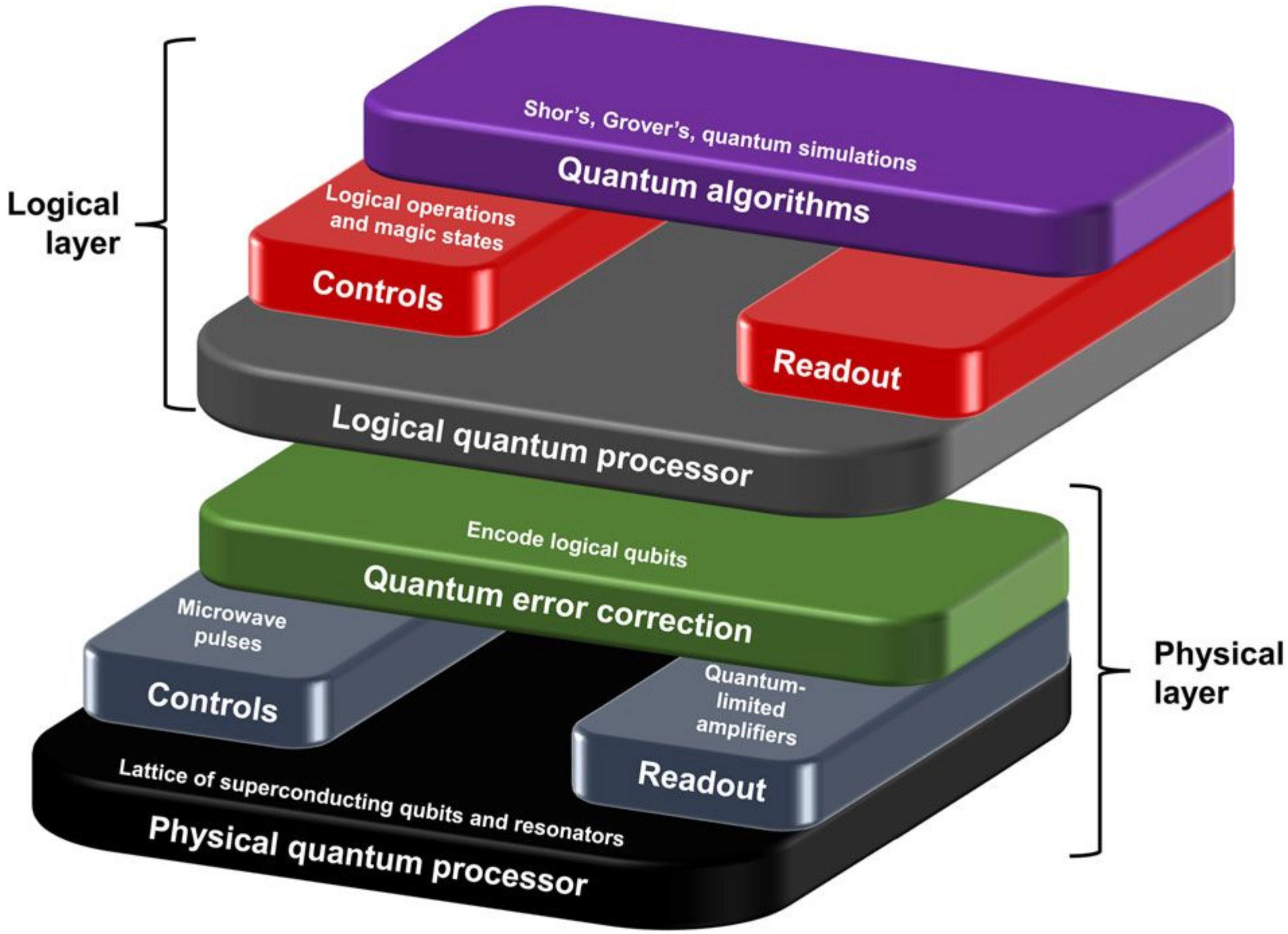
Each logical qubit requires thousands of physical qubits

Quantum Computing Stack

Industry Application

Quantum Algorithm

Quantum Compiler



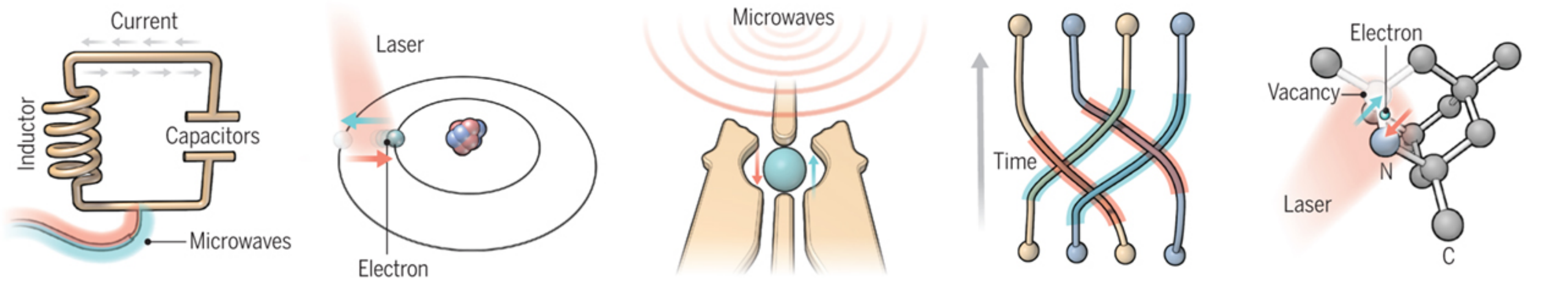
Quantum Error Correction

Control System

Quantum Hardware

Quantum computing: hardware platform

In the race to build a quantum computer, companies are pursuing many types of quantum bits, or qubits, each with its own strengths and weaknesses.



	Superconducting loops	Trapped ions	Silicon quantum dots	Topological qubits	Diamond vacancies
	A resistance-free current oscillates back and forth around a circuit loop. An injected microwave signal excites the current into super-position states.	Electrically charged atoms, or ions, have quantum energies that depend on the location of electrons. Tuned lasers cool and trap the ions, and put them in superposition states.	These "artificial atoms" are made by adding an electron to a small piece of pure silicon. Microwaves control the electron's quantum state.	Quasiparticles can be seen in the behavior of electrons channeled through semi-conductor structures. Their braided paths can encode quantum information.	A nitrogen atom and a vacancy add an electron to a diamond lattice. Its quantum spin state, along with those of nearby carbon nuclei, can be controlled with light.
Longevity (seconds)	0.00005	>1000	0.03	N/A	10
Logic success rate	99.4%	99.9%	~99%	N/A	99.2%
Number entangled	9	14	2	N/A	6
Company support	Google, IBM, Quantum Circuits	ionQ	Intel	Microsoft, Bell Labs	Quantum Diamond Technologies
Pros	Fast working. Build on existing semiconductor industry.	Very stable. Highest achieved gate fidelities.	Stable. Build on existing semiconductor industry.	Greatly reduce errors.	Can operate at room temperature.
Cons	Collapse easily and must be kept cold.	Slow operation. Many lasers are needed.	Only a few entangled. Must be kept cold.	Existence not yet confirmed.	Difficult to entangle.

Other platforms
- Photonic
- Atomic
- NMR
- …

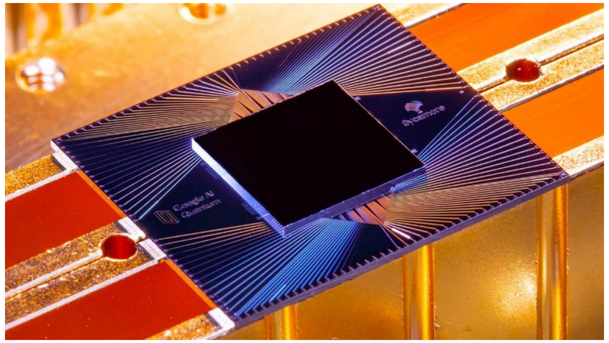
Core Metric
- Scalability
- Fidelity

Core Dilemma
- Easy to control
- Hard to be affected

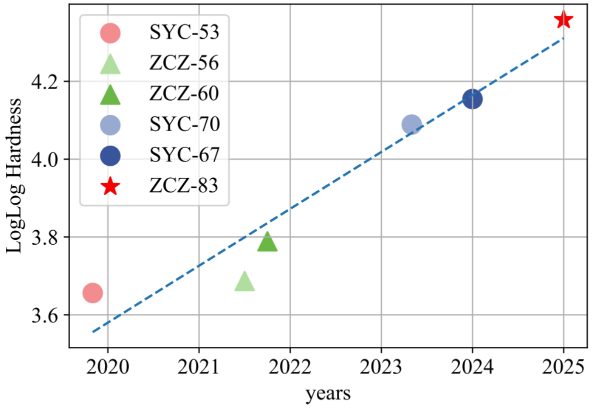
Quantum Computing: Where are we

- *Post classical Moore's Law*

- *Pre Quantum Moore's Law*



Vision: **double exponential**

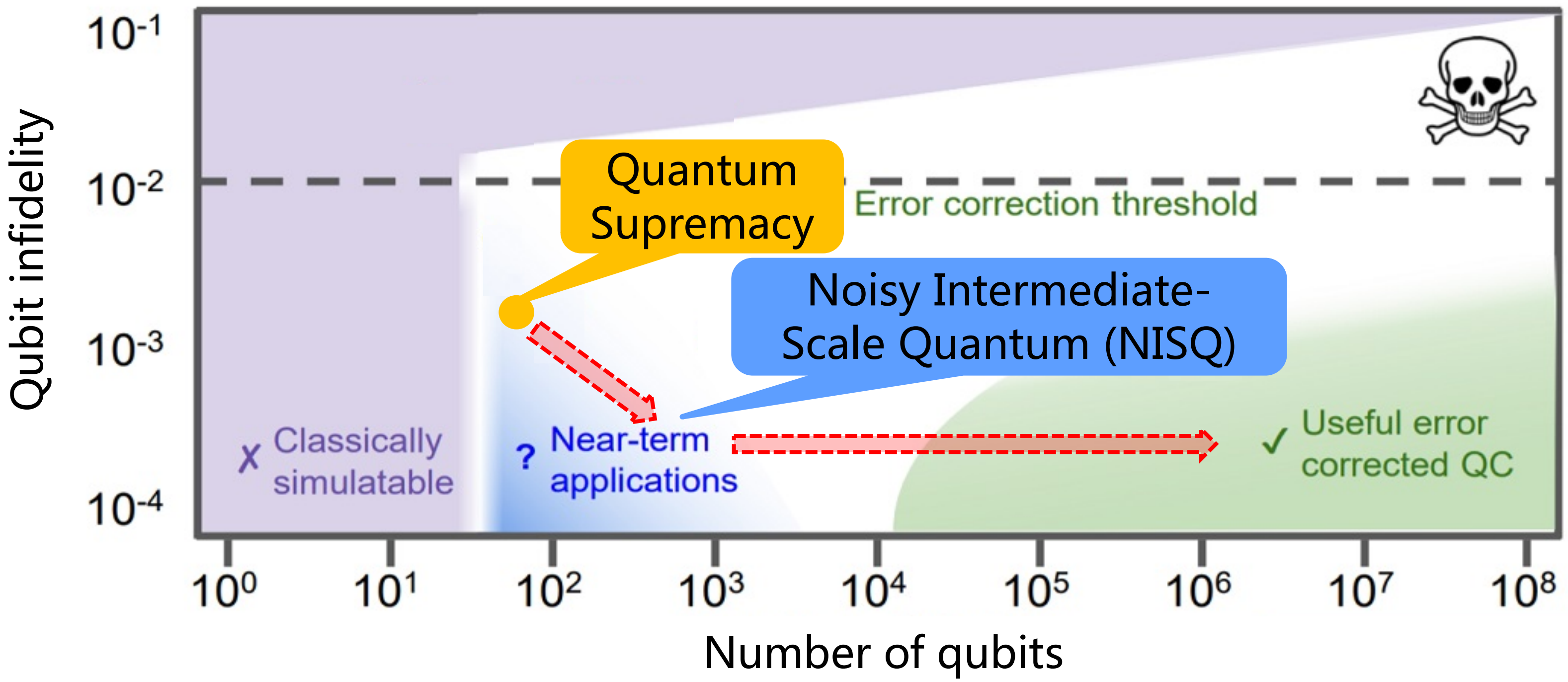


arXiv:2412.11924

3

Noisy Intermediate Scale Quantum (NISQ)

Quantum Computing: Paradigm shift



John Preskill @ Caltech

Define the stage: Quantum Supremacy & NISQ

Preskill 2012
Preskill 2018

Focus

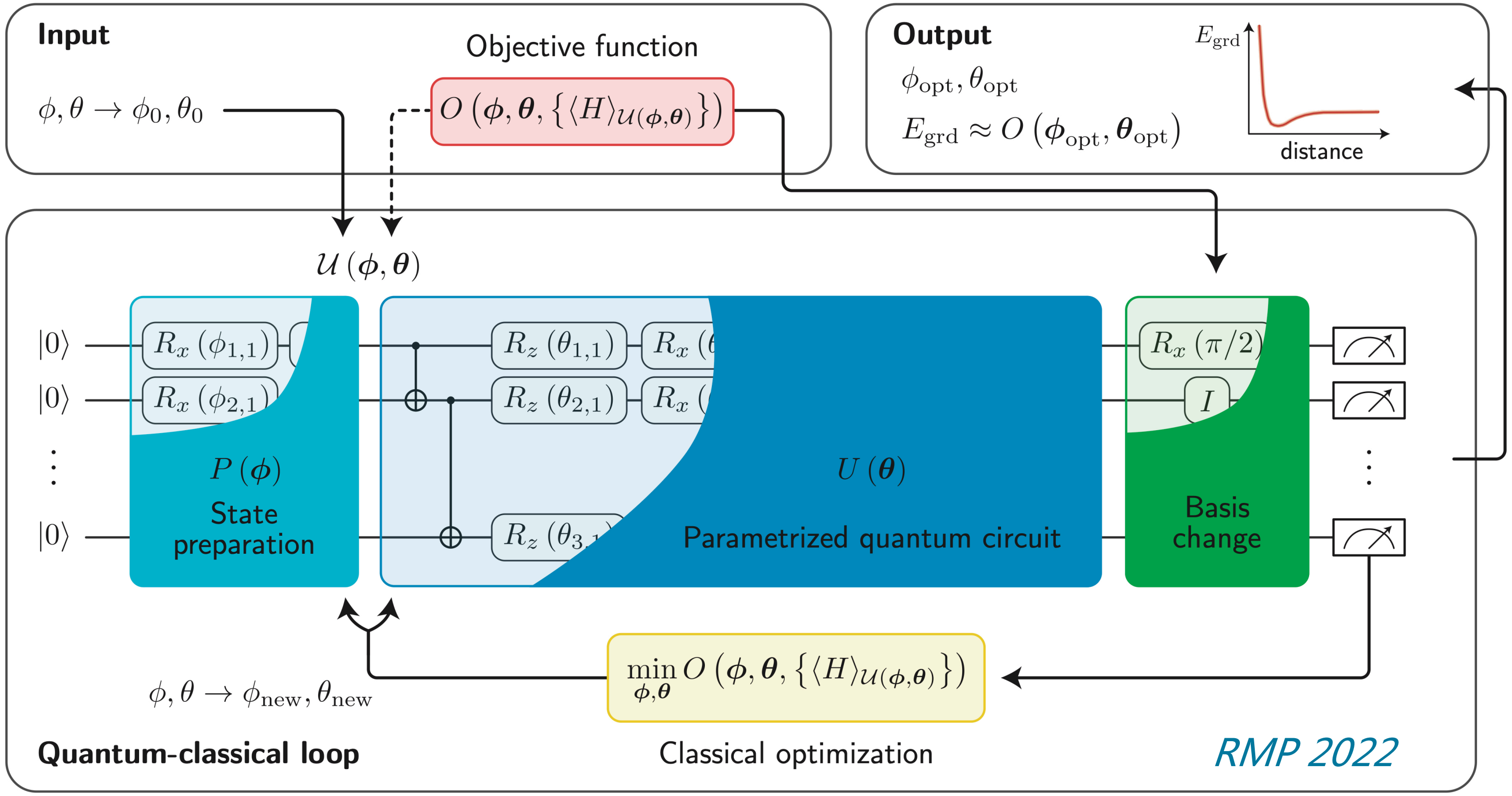
- Qubit building: quality first ↣ quantity first
- Driven force: academic ↣ academic + industry
- Role: universal CPU ↣ heterogeneous QPU
- Algorithms: Grover/Shor ↣ Variational Quantum Algorithms (VQA)
- Quantum noise: Quantum Error Correction (QEC) ↣ Mitigation (QEM)

Quantum Computing: Paradigm shift

	1990s	2020s
Classical computation paradigm	Universal computation from Turing and Neumann	Heterogeneous computing; Cloud computing; Special purpose computation
Computer Hardware	Burst of PC and CPU	Post Moore Law, burst of GPU/TPU/FPGA
Main problem/setup	Physics simulation based on differential equations	Large scale variational optimization for deep learning
New proposals on quantum computation	Feynman: Simulating quantum physics on a quantum computer	Preskill: Quantum Supremacy and NISQ
Quantum computation paradigm	Universality and fault tolerance of quantum computation	Quantum classical hybrid computation scheme; Quantum error mitigation
Vision of quantum computer	Universal CPU at home	Specific tailored QPU on the cloud
Quantum Algorithms	Shor, Grover	VQA: QAOA, VQE, etc.

Variational Quantum Algorithm

Framework



Quantum-Classical Hybrid Scheme

Inspired by **deep learning** setup

Applications :

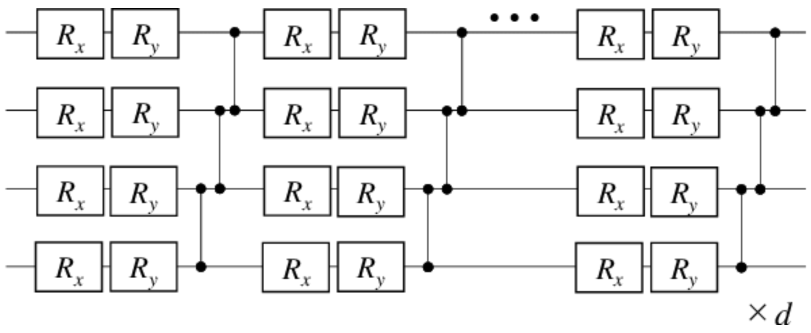
- Quantum simulation
- Combinatorial optimization
- Machine learning

Challenges :

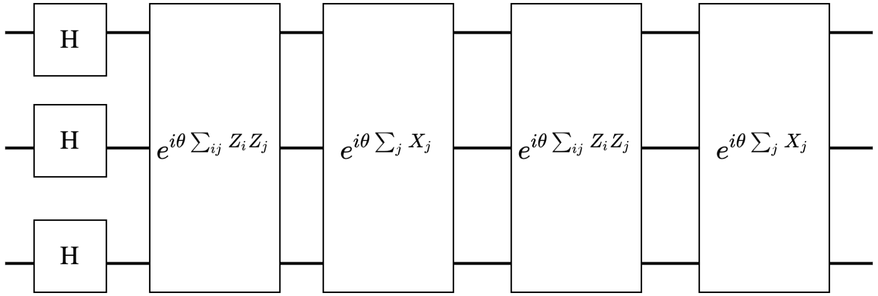
- Circuit ansatz design
- Quantum error mitigation
- Barren plateau
- Measurement efficiency

Channllenges 1: Ansatz Design

Common circuit ansatz



Hardware efficient ansatz *IBM 2017*



QAOA ansatz *Farhi 2014*

$$|\Psi(\theta)\rangle = \mathrm{e}^{\hat{\mathrm{T}}(\theta)-\hat{\mathrm{T}}^{\dagger}(\theta)}|\Psi_0\rangle$$

Unitary-coupled cluster *Narkoutsos et al. 2018*

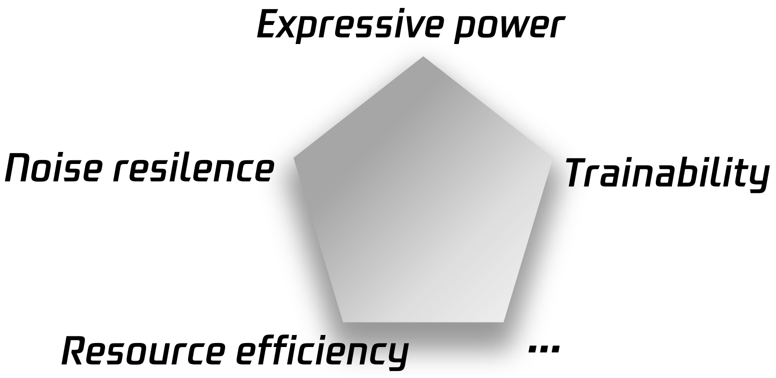
$$|\Psi(\theta)\rangle = \prod_{\mathrm{k}=1}^{\mathrm{N}} \mathrm{e}^{-\mathrm{i}\theta_{\mathrm{k}}\hat{\mathrm{P}}_{\mathrm{k}}/2}|\Psi_0\rangle$$

Qubit-coupled cluster *Ryabinkin et al. 2018*

Tensornetwork inspired
Adiabaticity inspired
Hamiltonian inspired
Neural network inspired
……

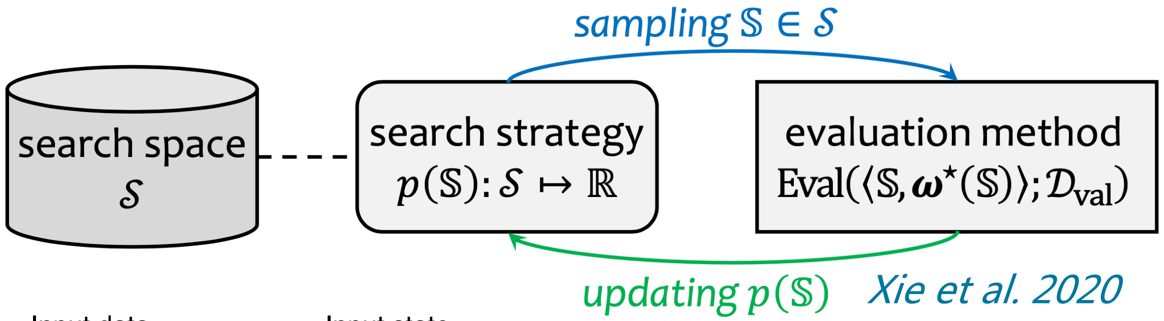
QAS

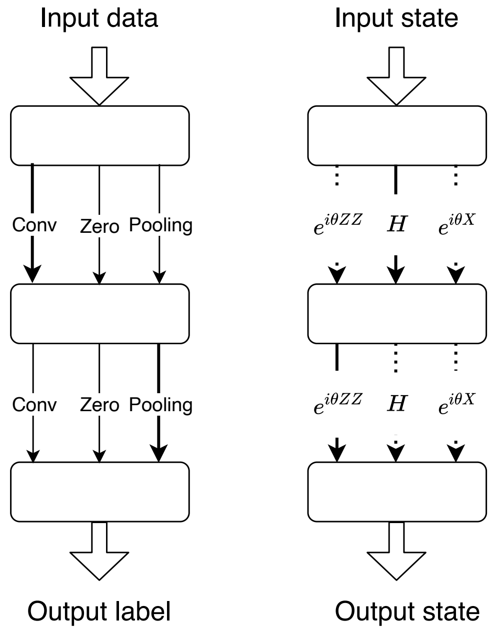
?



Differentiable Quantum Architecture Search

Inspired by NAS





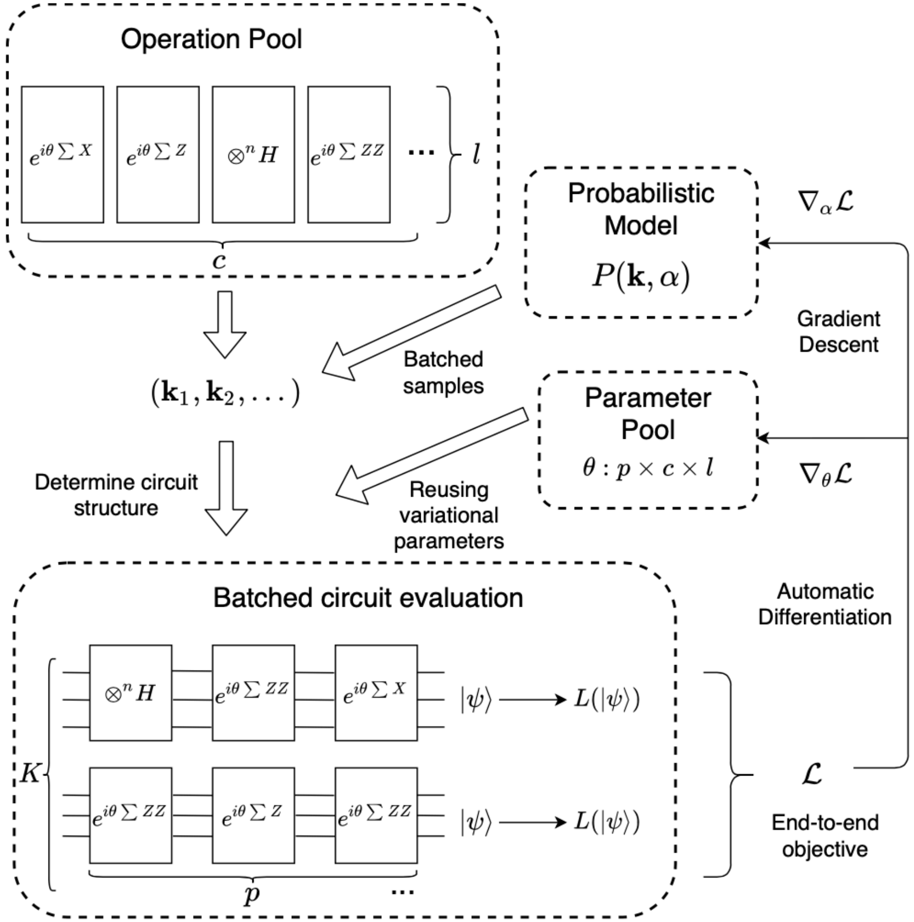
(a) DARTS (b) DQAS

From DARTS to DQAS :

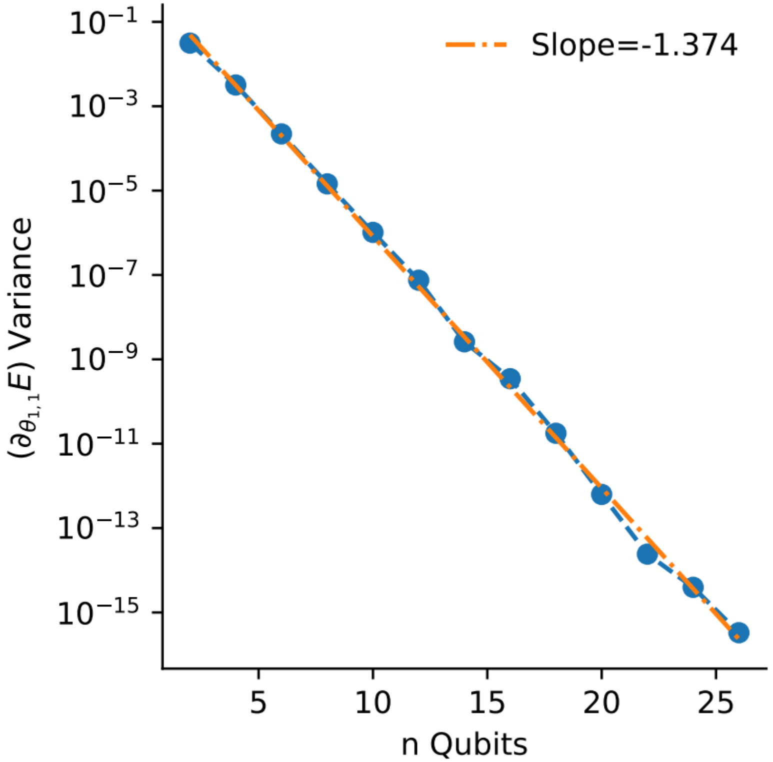
Replace weighted sum with probability sampling to keep unitary nature

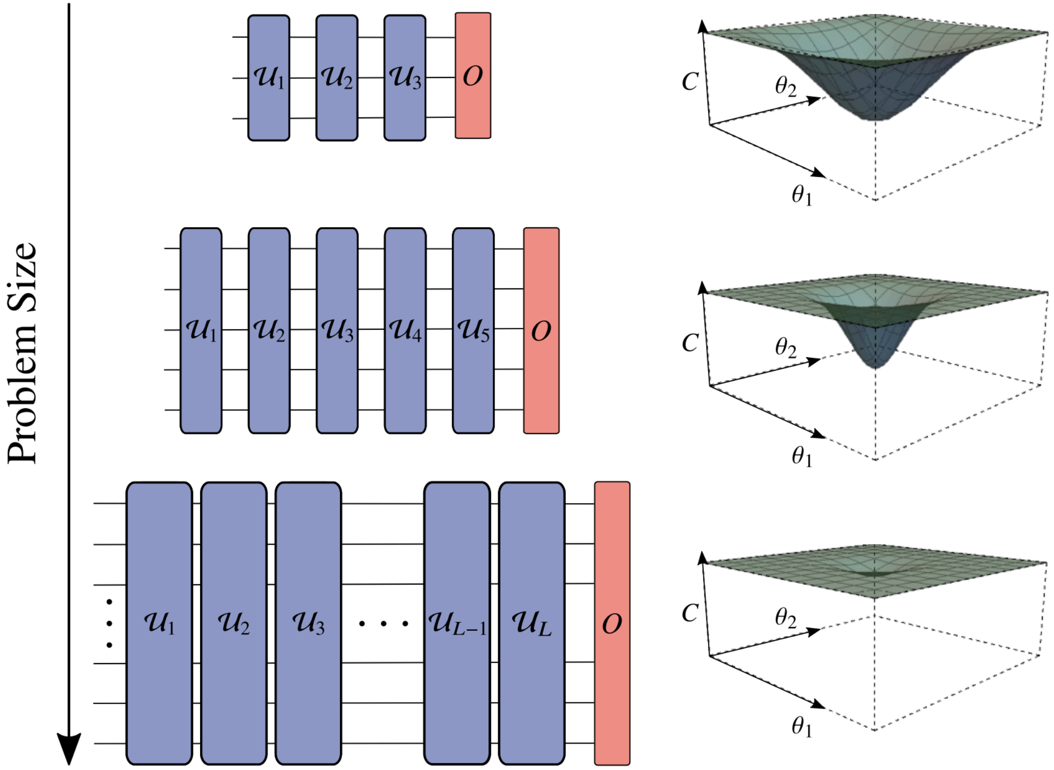
__S.-X. Zhang__, et al. QST 7, 045023 (2022)

DQAS workflow



Challenges 2: Optimization problem



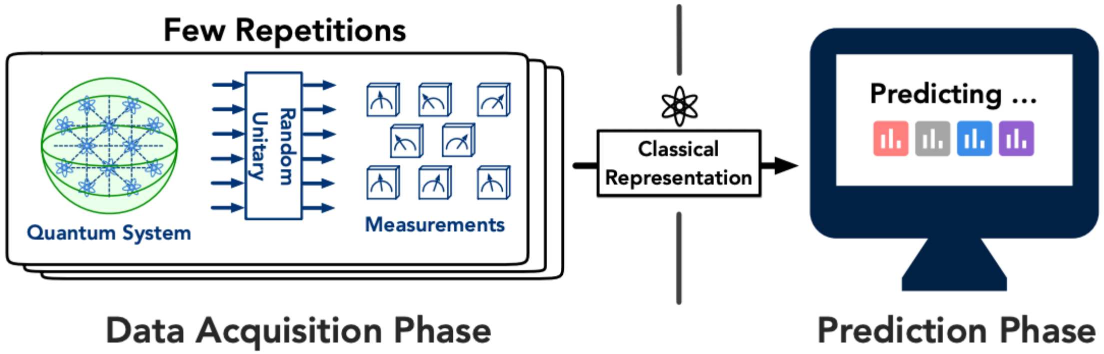


Barren plateau:
Quantum Gradient Vanishing

Nat. Comm. 9, 4812 (2018)

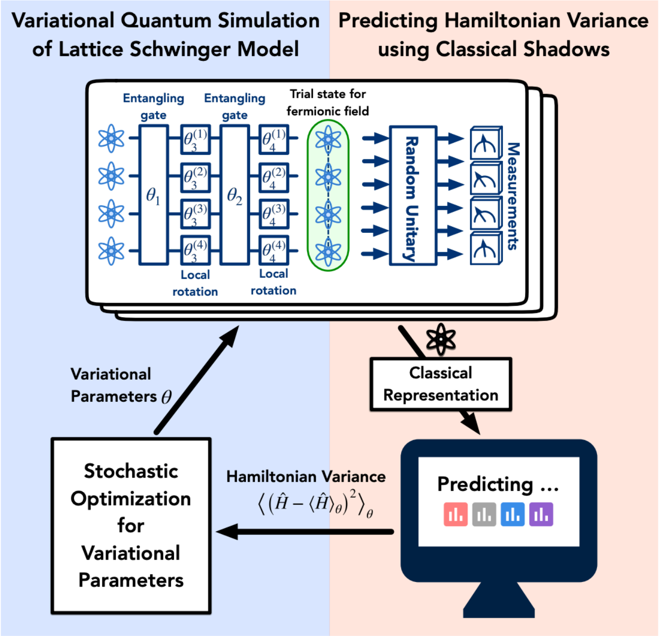
BP is very common in VQA:
Increasing qubit number, quantum noise, quantum entanglement can all lead to BP

Challenges 3: Measurement Efficiency



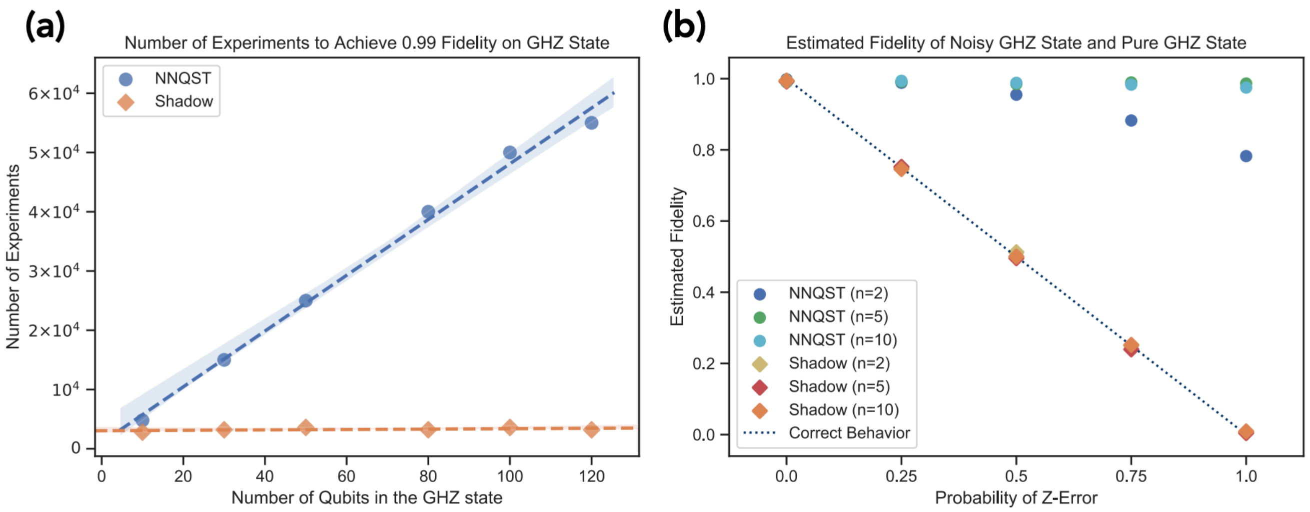
Possible Properties

- Quantum Fidelity
- Entanglement Witness
- Entanglement Entropy
- 2-point Correlations
- Hamiltonian
- Local Observables



Random classical shadow: Measure once, compute all

Nat. Phys. 16, 1050 (2020)



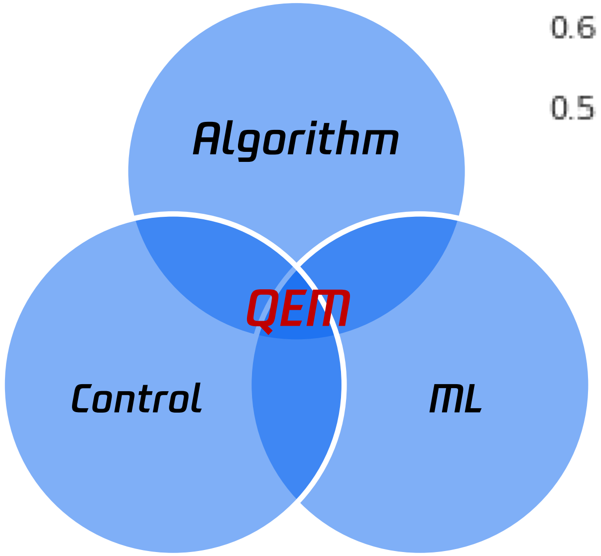
Challenges 4: Error mitigation

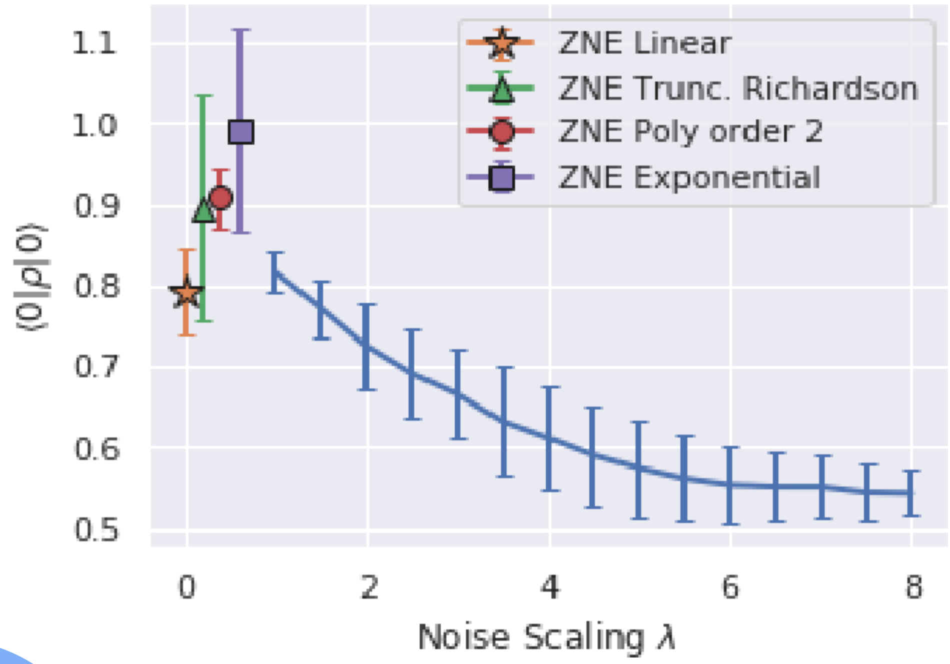
Quantum Error Correction ↣ Quantum Error Mitigation (QEM)

- GRAPE：波形优化
- DD：动态解耦
- ZNE：零噪声延拓
- QP：准概率分解
- VD：虚拟蒸馏
- CDR：Clifford 数据回归
- SV：对称性检验
- REM：读取噪声消除
- RC：随机编译

Hardware level

Software level



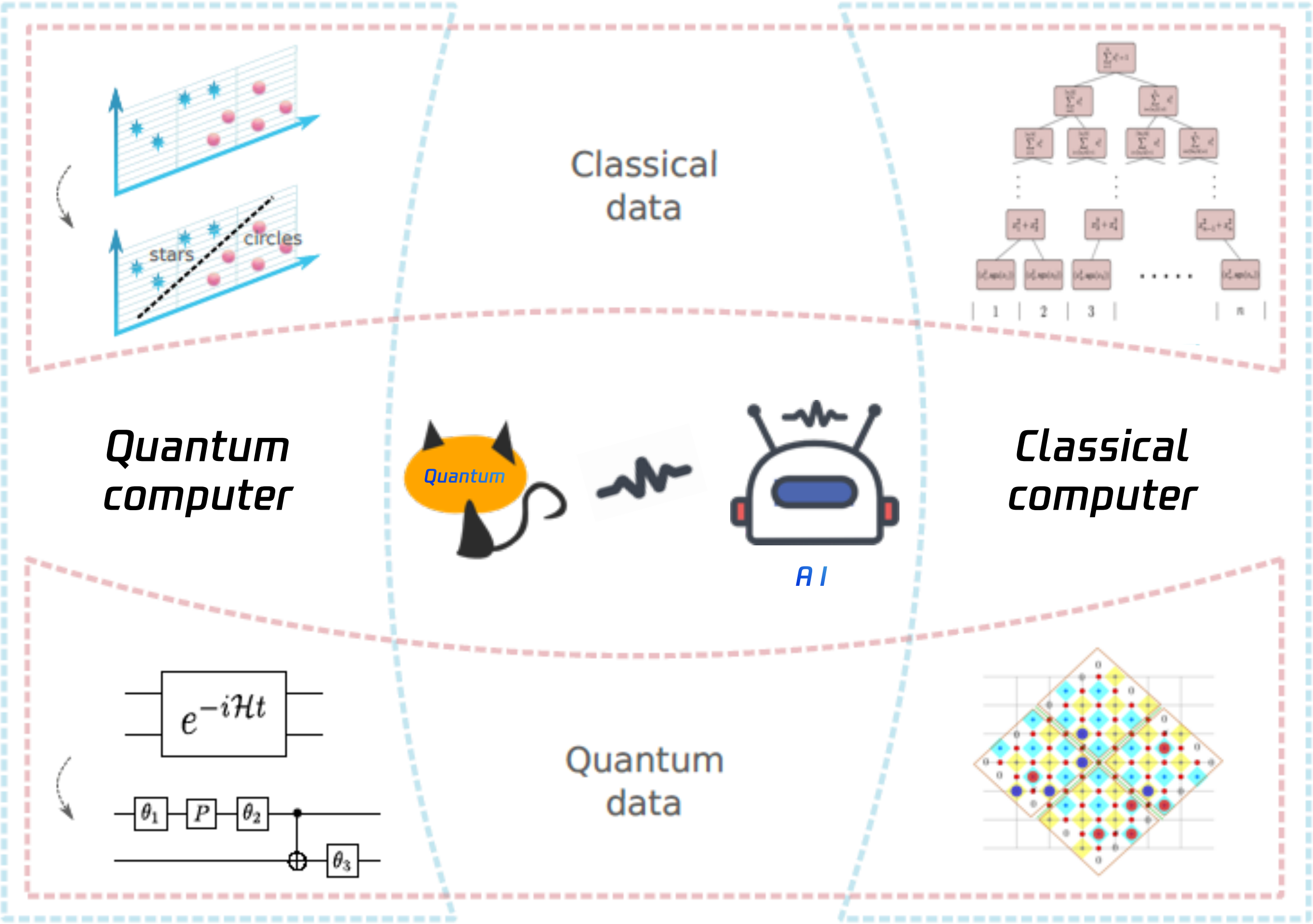


ZNE example

Quantum Machine Learning

Quantum Computing Engine for ML

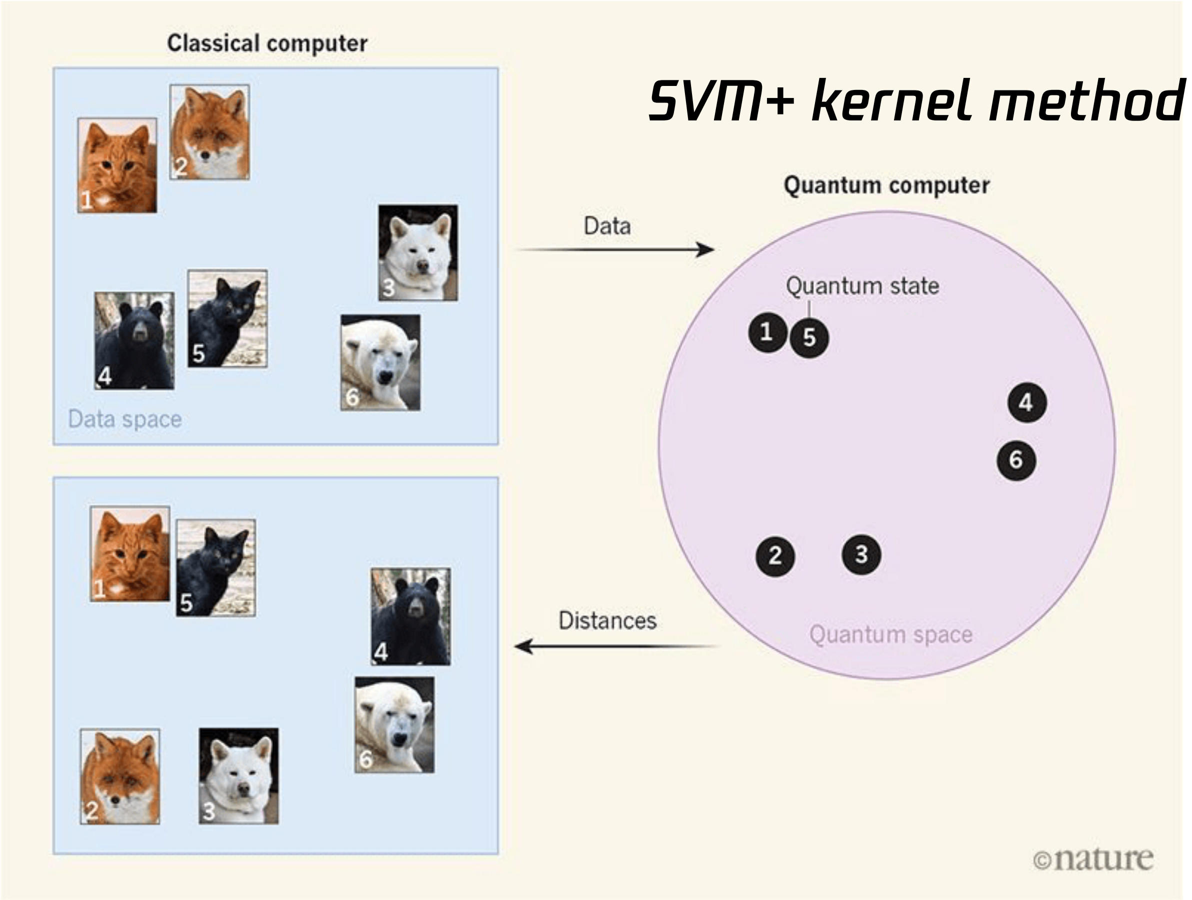
Quantum inspired ML



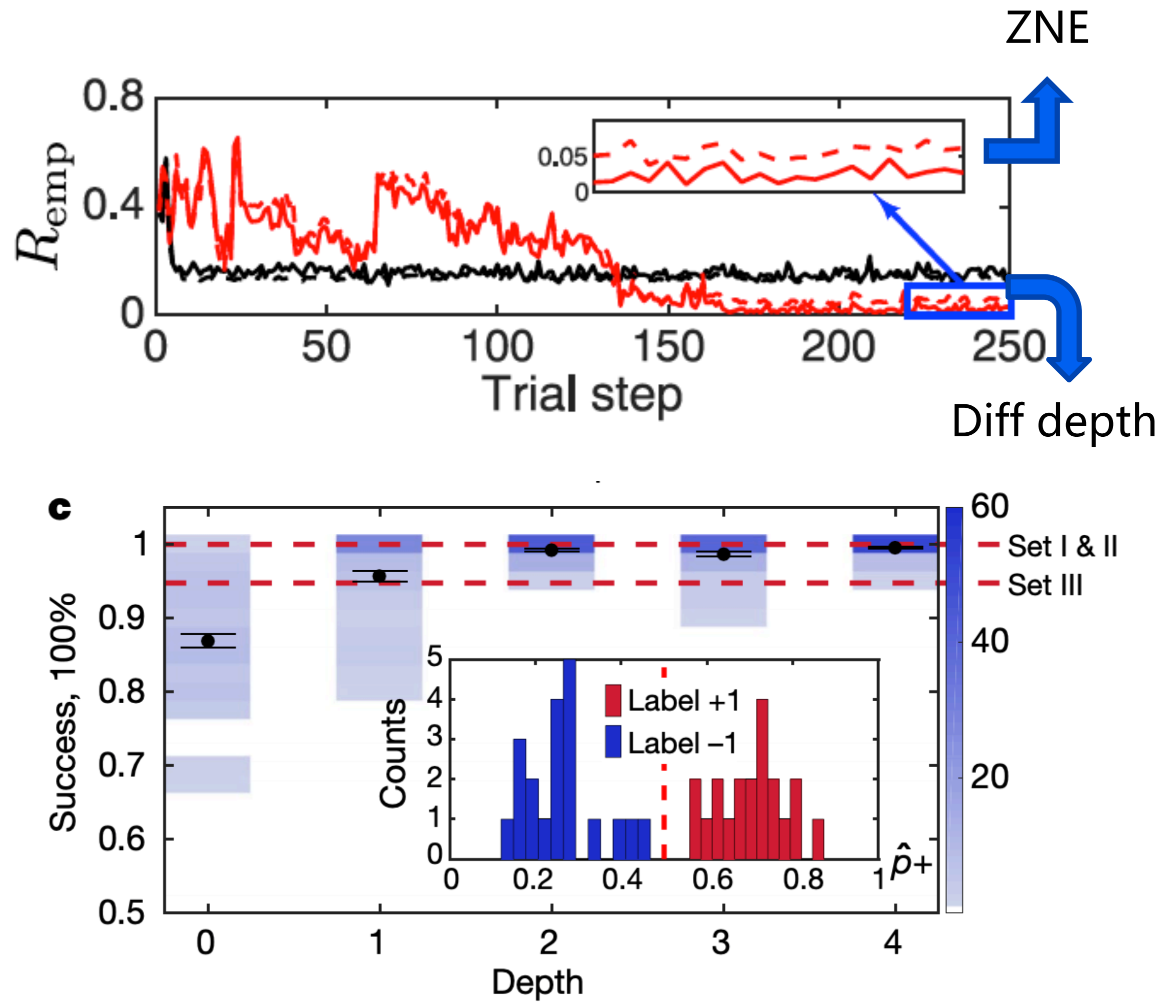
ML assisted quantum simulation

ML on quantum physics

Classfication on IBMQ

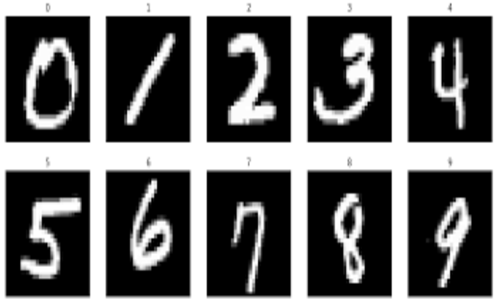


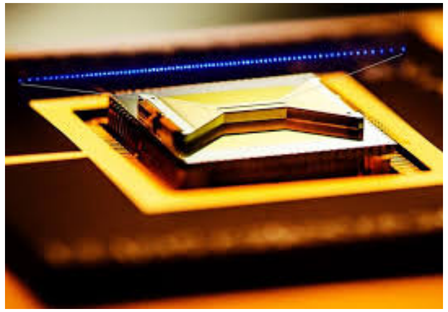
SVM+ kernel method

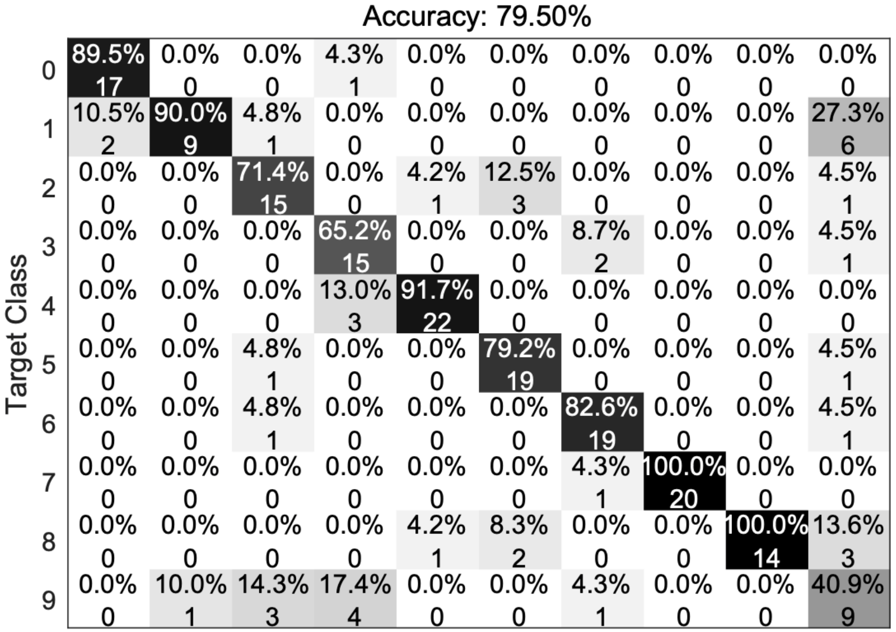


Nature 567, 209 (2019)

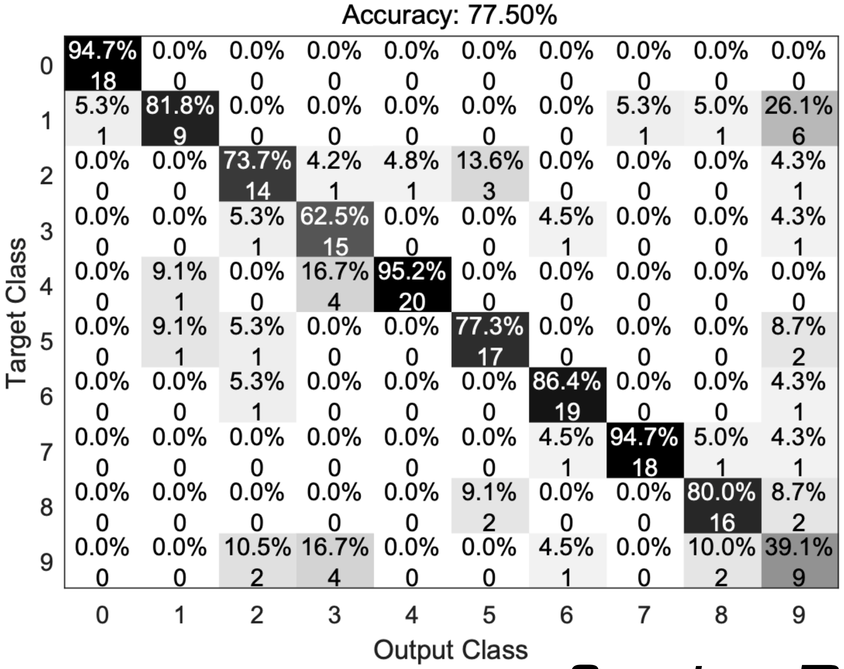
Classification on IonQ







Classical ML



Quantum ML

arXiv:2012.04145

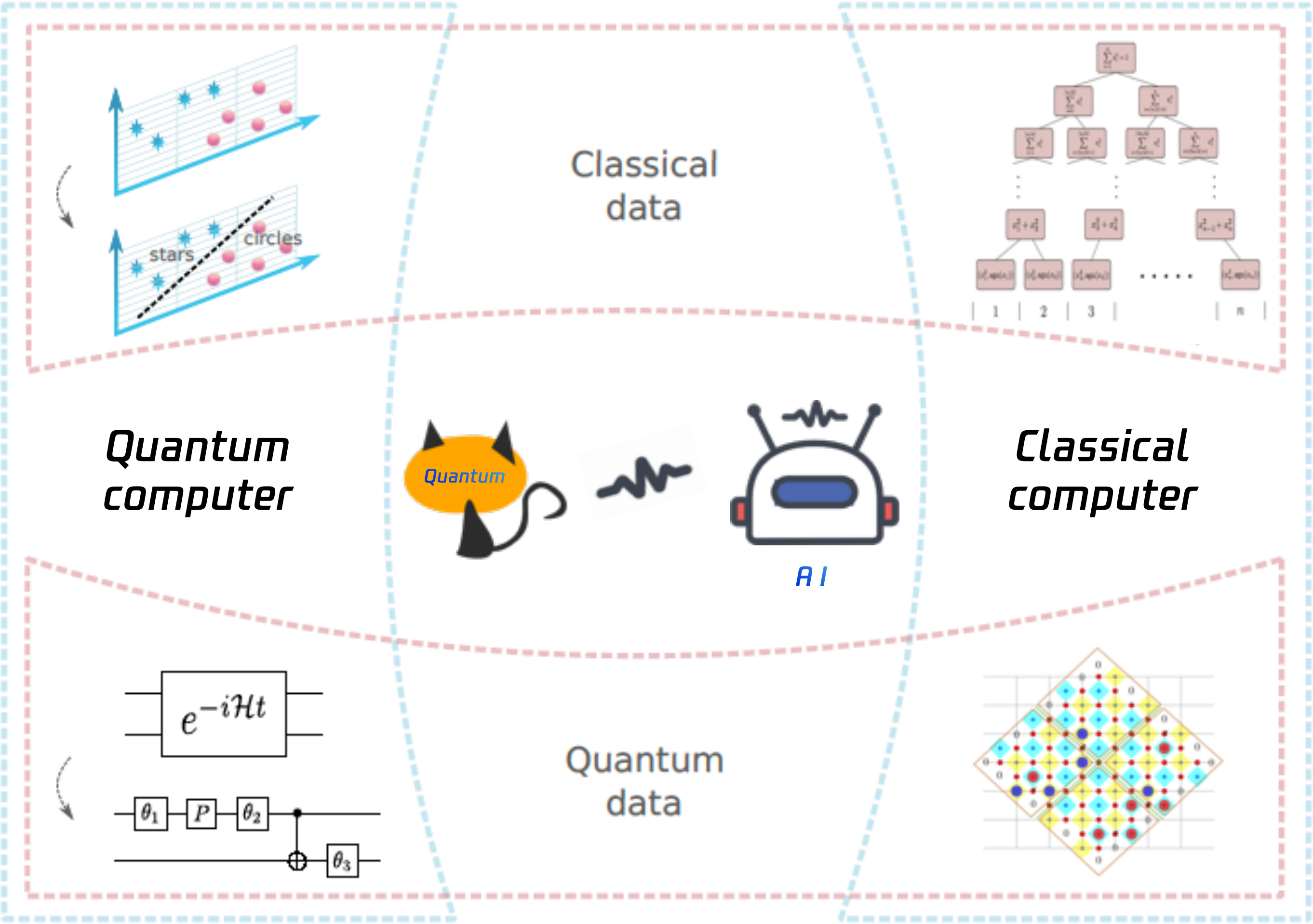
11-qubit experiment with 10-class classifications

Nearest centroid classification

Quantum Machine Learning

Quantum Computing Engine for ML

Quantum inspired ML



ML assisted quantum simulation

ML on quantum physics

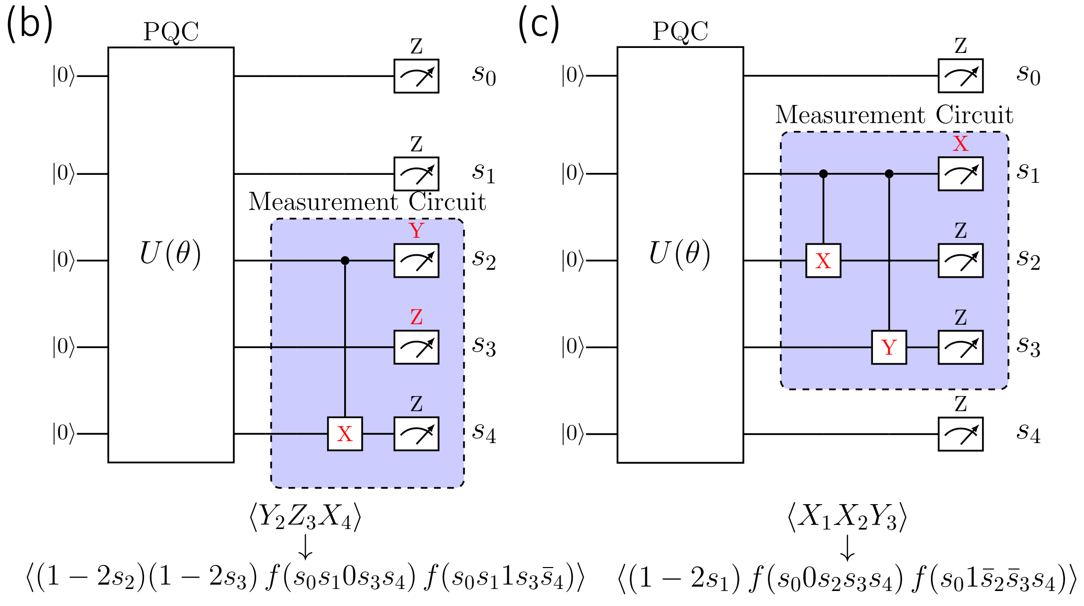
VQNHE: Neural post-processing

Neural enhanced quantum state

- Flexible
- General & Powerful

$$\hat{f} = \sum_{s\in\{0,1\}^n} f_\phi(s)\,|s\rangle\langle s|\,,\ \ |\psi_f\rangle = \hat{f}\,|\psi\rangle$$

Numerical simulation is okay,
but how about the experiments?



Measurement Circuit

- Build measurement circuit for each Pauli string!
  - Select the star(0) qubit (with X or Y)
  - CX/Y/Z on qubits in the same Pauli string
  - Measure X/Y on the star qubit,
    and Z on other qubits as bitstring s
- Complex valued neural network is also supported with a similar generalization

$$\langle \hat{H}\rangle_f = \frac{\langle \psi_f|\,\hat{H}\,|\psi_f\rangle}{\langle \psi_f|\psi_f\rangle}$$

$$\langle \hat{H}\rangle_{\psi_f} = \frac{\langle (1-2s_0) f(0 s_{1:n-1}) f(1\widetilde{s_{1:n-1}})\rangle_{UV}}{\langle f(s)^2\rangle_U}$$

***S.-X. Zhang**, et al. PRL 128, 120502 (2022)*

VQNHE workflow

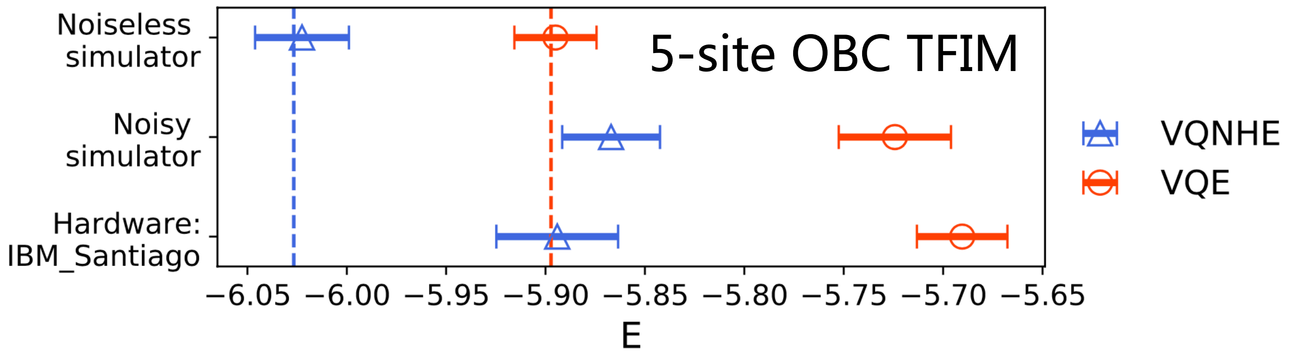
***S.-X. Zhang**, et al. PRL 128, 120502 (2022)*

- ***1D spin models***

12 sites, PBC

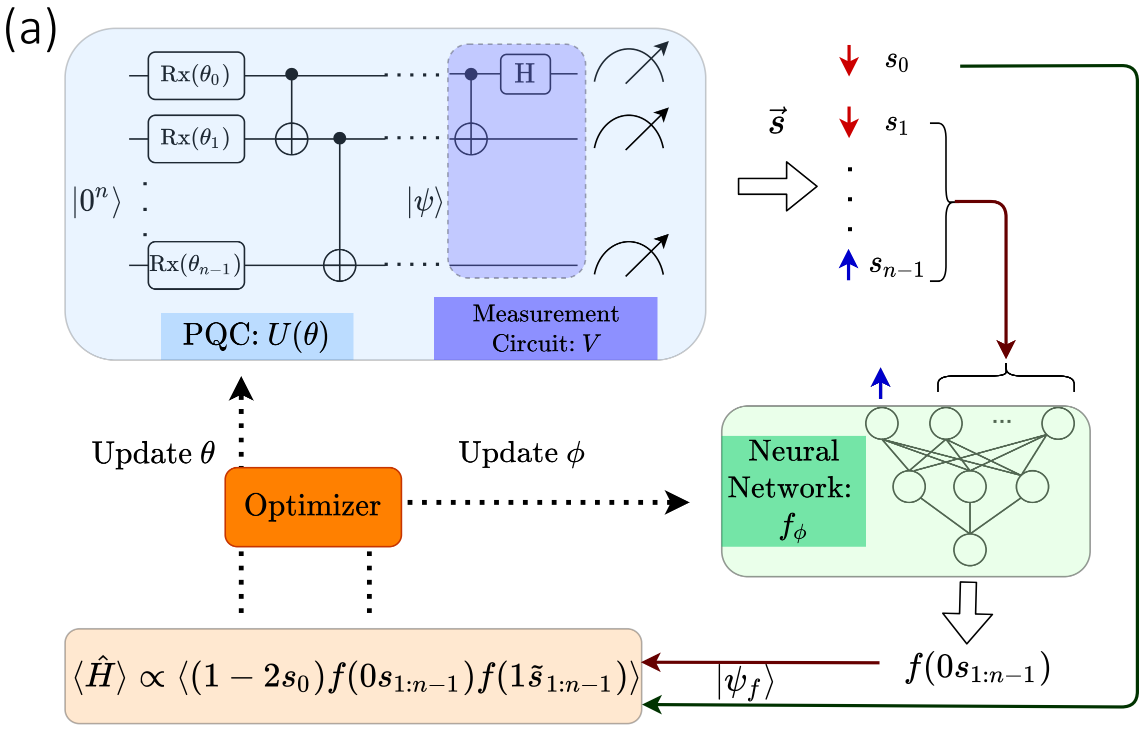
Model	TFIM	Heisenberg Model
VQE	-14.914 $(3 * 10^{-2})$	-21.393 $(7 * 10^{-3})$
VQNHE	-15.319 $(2 * 10^{-4})$	-21.546 $(2 * 10^{-4})$
exact	-15.3226	-21.5496

- ***Adaptive Noise Resilience***



Hardware results

***S.-X. Zhang**, et al. AQT (2023)*

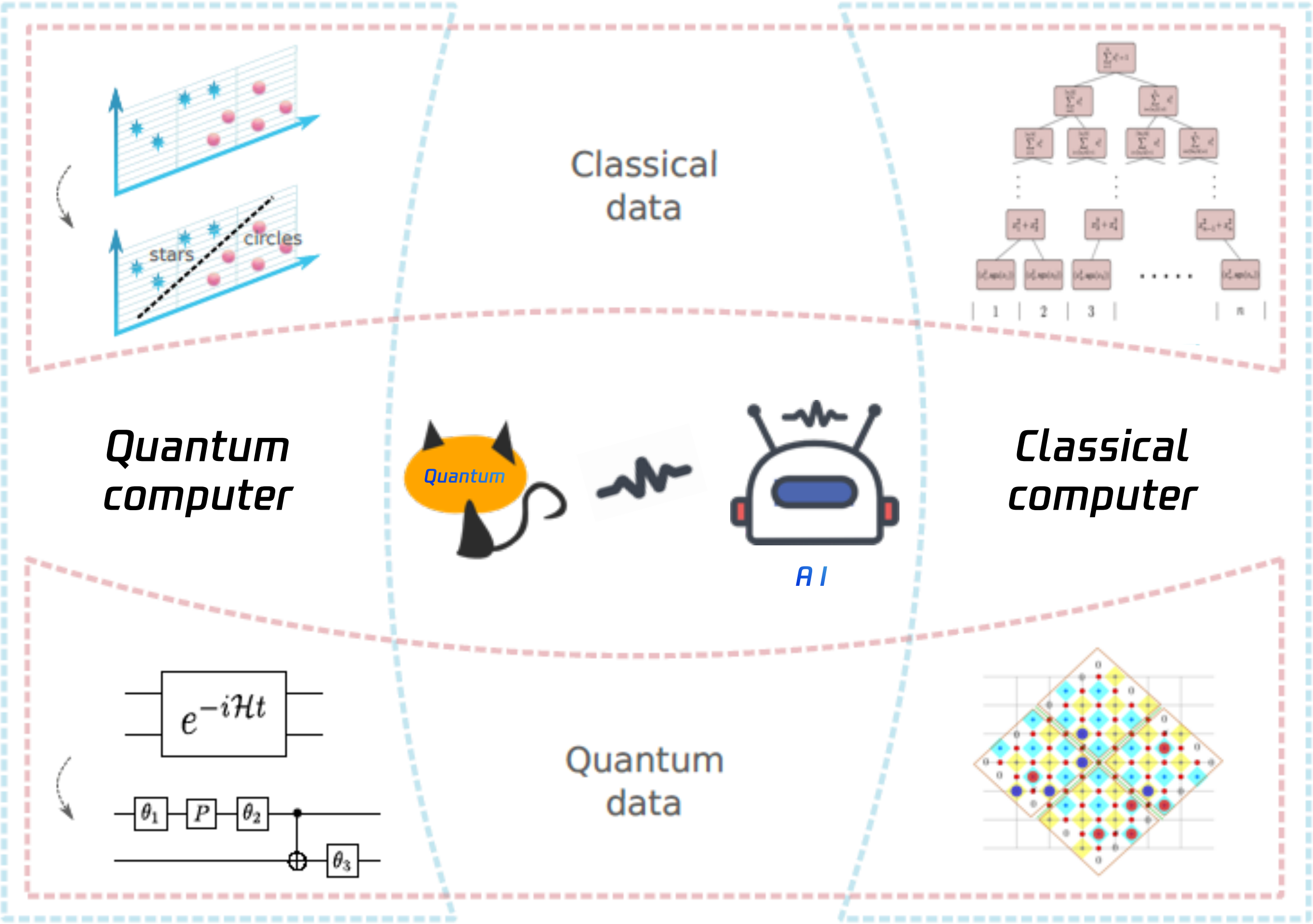


Variational quantum-neural hybrid eigensolver

Quantum Machine Learning

Quantum Computing
Engine for ML

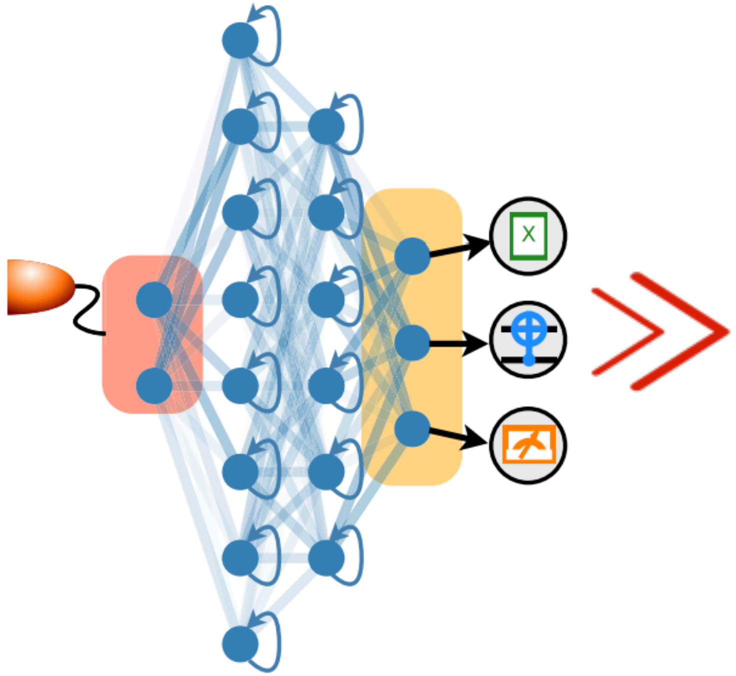
Quantum inspired ML



ML assisted
quantum simulation

ML on
quantum physics

AI guided error correction

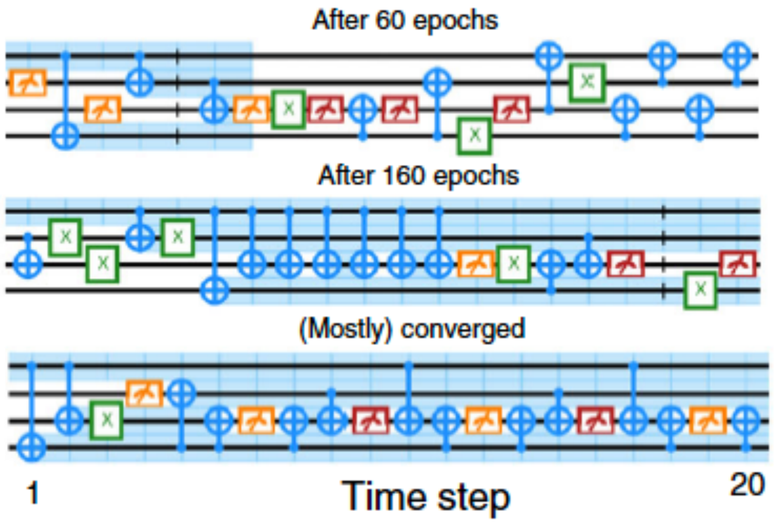


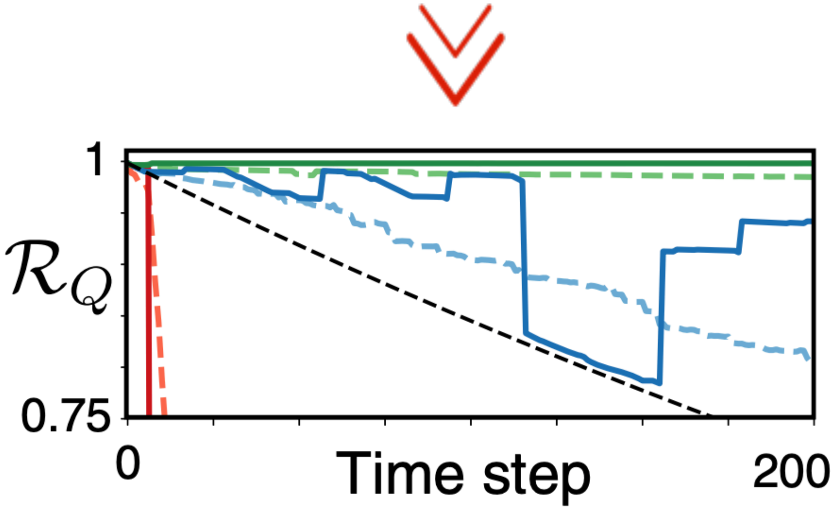
Recurrent network

Measurement results

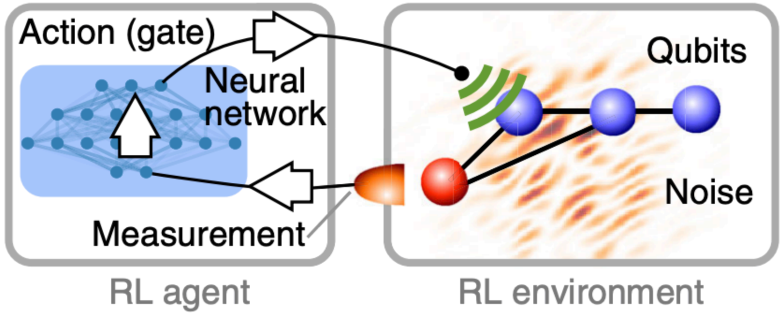
Action probabilities

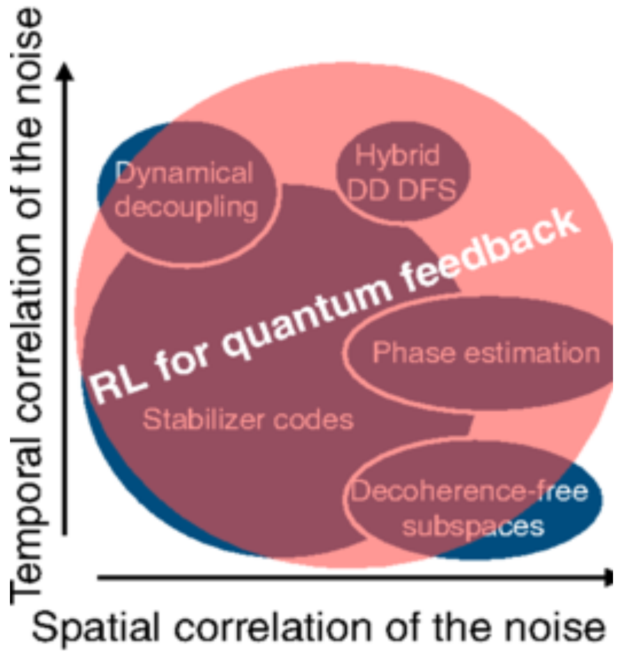
Phys. Rev. X. 8, 031084 (2018)



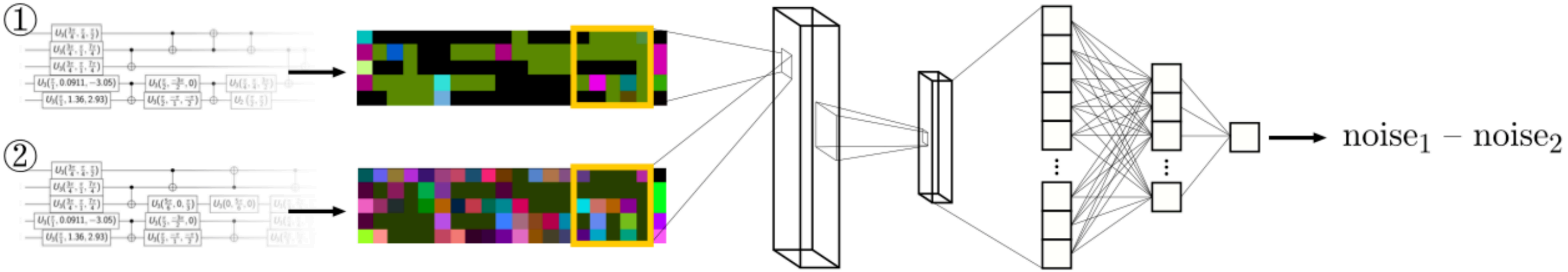


RL guide the circuit design

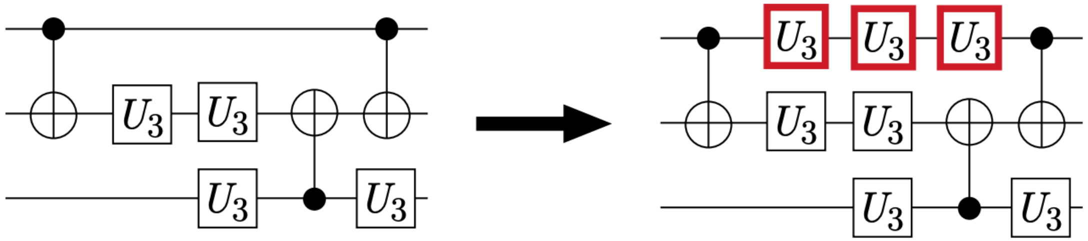




AI guided error correction



CNN determine the noisy effect of each circuit



Policy : dynamical decoupling

Device	Δ Noise (Burl.)	Δ Noise (Lond.)
Burlington	**11% [10%, 12%]**	10% [8%, 11%]
Burl. random	4.5% [4.4%, 4.6%]	4.5% [4.4%, 4.6%]
Essex	4% [3%, 5%]	4% [2%, 5%]
London	5% [4%, 6%]	**13% [13%, 14%]**
Lond. random	7.3% [7.2%, 7.5%]	7.3% [7.2%, 7.5%]
Ourense	6% [5%, 7%]	7% [6%, 8%]
Vigo	4% [4%, 5%]	3% [2%, 4%]
Yorktown	6% [5%, 7%]	4% [3%, 5%]

Error correction results

arXiv:2005.10811

4 Quantum Software

Quantum software: Background

- ## Quantum Software

Qiskit — IBM

Cirq — Google

<Q#> — Microsoft

Amazon Braket — AWS

NISQ Challenges

Variational

Machine learning

Efficiency

- ## Next Generation Quantum Software

NISQ Friendly

Differentiable

ML interface

GPU support

1.5 Gen

飞桨 Quantum — Non auto-differentiable, Fixed interface

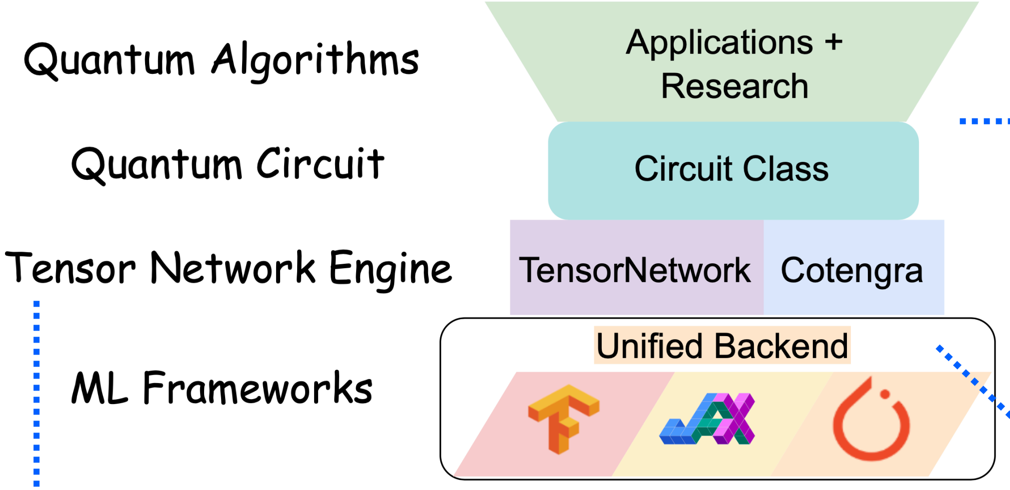
TensorFlow Quantum — No GPU support, Fixed interface

PENNY LANE — Batch on trainable weights, Too slow

2 Gen?

TensorCircuit-NG: Overview

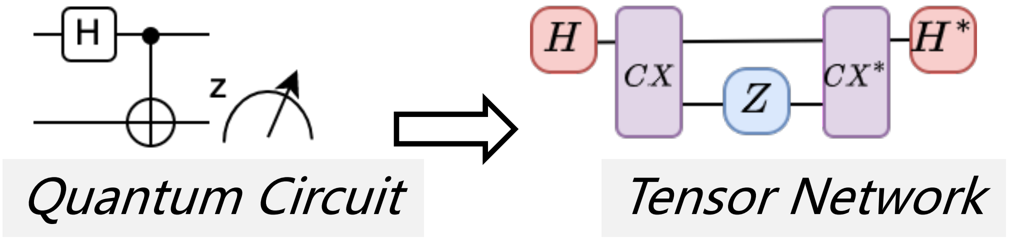
Quantum Circuit Simulation Software Framework



TenCirChem JCTC 2023

- Quantum computing chemistry package
- UCC/HEA ansatz for electronic structure, noisy circuit, variational dynamics…

- Tensor network contraction engine
- Enable large-scale simulation for shallow ansatz, TN based/inspired ansatz, QCNN…



- Unified Frameworks: TensorFlow, Jax, PyTorch
- Unified Paradigm: AD, JIT, VMAP
- Unified Devices: CPU, GPU, QPU

S.-X. Zhang *et al, Quantum 2023*

TensorCircuit-NG: Advantage

TensorCircuit
Next Generation

Efficiency

- Optimized contraction path
- Hardware acceleration
- Just-in-time compilation
- Parallelism in different levels
- Innovation on algorithms
- Advanced automatic differentiation

Acceleration ⇒

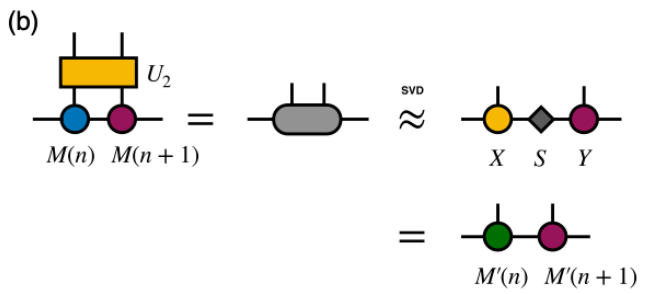
- Qiskit
- Pennylane
- TFQ

- VQE task : **10x**
- QML task : **100x**
- Variational dynamics : **1000x**
- Hamiltonian expectation : **80000x**
- Hessian matrix : **200000x**
- Qubits support in 1D task : **600+**

MPS/MPO support

- Support MPS as input state
- Support MPO as gate or observable
- MPS-TEBD approximate simulation

Y. Zhou et al. PRX 2020



Analog simulation

- Support digital/analog hybrid simulation for pulse control and neural atom platforms

***S.-X. Zhang** et al, Quantum 2023*

TensorCircuit-NG: AD

AD for wavefunction

- Any quantity derived from wavefunction is differentiable

AD with SVD

arXiv:1909.02659

- MPS Simulator and two-qubit gate decomposition is differentiable

AD on noise parameters

- Noise model is differentiable

AD on circuit structure

- Circuit structures is differentiable via DQAS

AD on neural weights

- Classical part is jointly differentiable

Various backend agnostic API

`grad`	`jvp`
`value_and_grad`	`vjp`
`jacfwd`	`hessian`
`jacrev`	`stop_gradient`
`qng`	`dynamics_rhs`

$$A_{ij} = \Re\left(\frac{\partial\langle\phi(\tau)|}{\partial\theta_i}\frac{\partial|\phi(\tau)\rangle}{\partial\theta_j}\right)$$

$$C_i = \Re\left(-\sum_a \lambda_a \frac{\partial\langle\phi(\tau)|}{\partial\theta_i} h_a|\phi(\tau)\rangle\right)$$

$$\boxed{\sum_j A_{ij}\dot{\theta}_j = C_i}$$

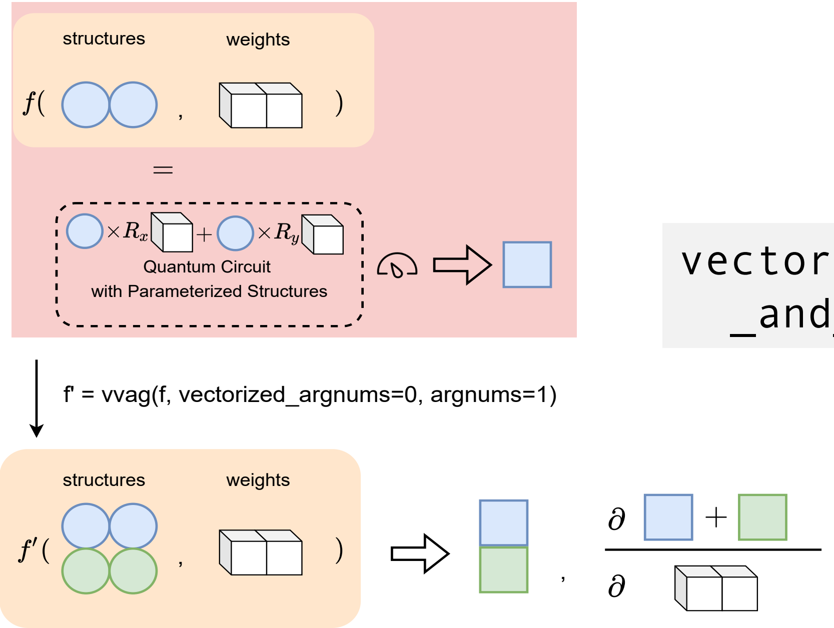
Super efficient variational dynamics implementation

Efficiency over parameter shift

- Gradient: O(1) vs O(n)
- Hessian: O(1) vs O(n^2)

TensorCircuit-NG: VMAP

- *VMAP input state* `Circuit(, inputs)`
  - Quantum Machine Learning
  - Quantum chaos

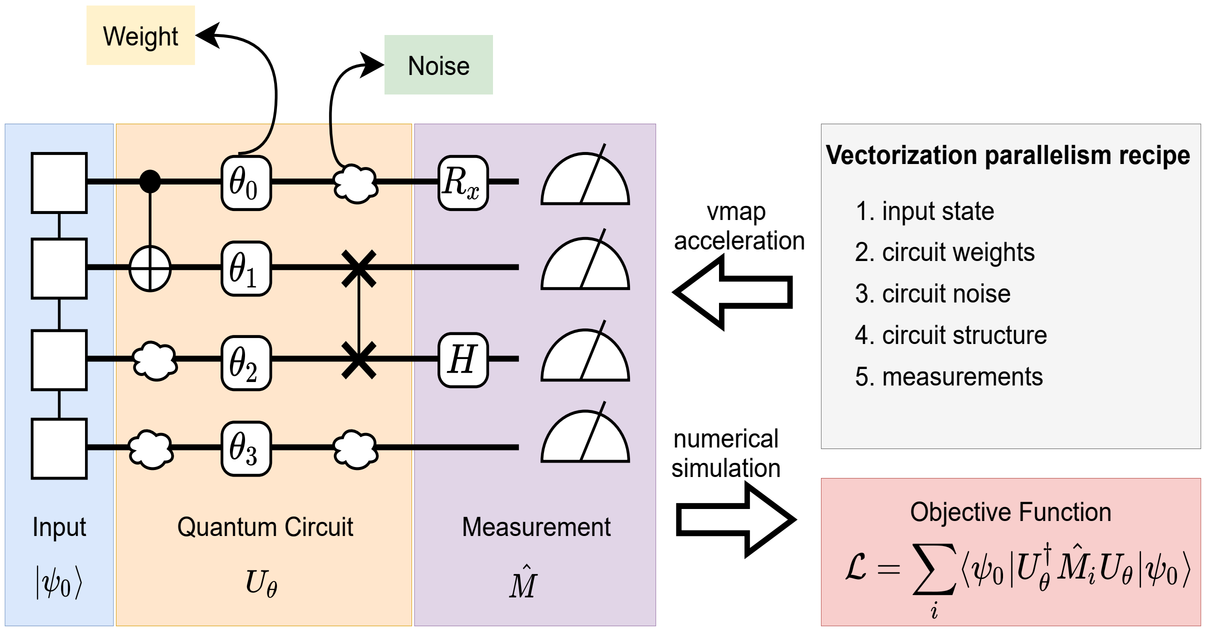


`vectorized_value_and_grad(f)`

- *VMAP circuit structure* `c.general_kraus(, status)`
  - Barren Plateau
  - Quantum Architecture Search
  - Monte Carlo Noise Simulation

- *VMAP circuit parameters* `c.exp1(,theta)`
  - Batched VQE
  - Barren Plateau
  - Parameter Shift

- *VMAP cost function* `parameterized_measurements(c, structures)`
  - Pauli string expectation



TensorCircuit Next Generation

TensorCircuit-NG: Ecosystem

Open source community

- GitHub: https://github.com/tensorcircuit/tensorcircuit-ng
- PyPI: `pip install tensorcircuit-ng`

Metrics

30+ tutorials	70+ examples	10+ benchmarks	1000 pages doc
20+ contributors	600k downloads	90 citations	300 stars/forks

Users

清华大学 Tsinghua University
北京大学 PEKING UNIVERSITY
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西湖大學 WESTLAKE UNIVERSITY
中国科学院数学与系统科学研究院 Academy of Mathematics and Systems Science Chinese Academy of Sciences
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CityU 香港城市大學 City University of Hong Kong
Institute of Physics CAS
HARVARD UNIVERSITY
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THE UNIVERSITY OF CHICAGO
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USC University of Southern California
Tulane University
NVIDIA
Google
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Tencent 腾讯
中国银行 BANK OF CHINA
中国工商银行 INDUSTRIAL AND COMMERCIAL BANK OF CHINA
平安银行 PING AN BANK
华大基因 BGI

Up to

10 ~ 10^6

times speed up
over industry standard software

World record

600+

qubits VQE workflow

Ecosystem

Community
+
Industry
+
Academic

Next Generation Quantum Software

Easy Access

`pip install` `docker pull`

TensorCircuit

4

machine learning frameworks makes one

GPU

support

Cloud

ready

30+

Jupyter tutorials

70+

Application examples

40+

pages whitepaper

10+

benchmarks

Up to

50%

code reduction for given tasks

90+

research projects related

Thanks