Quantum Leap : Harnessing Artificial Intelligence, Digital Twin Technology, and Quantum Computing for Next-Generation Simulation and Optimization

연세대학교 IT융합공학과

STL (Seamless Trans-X Lab)

김 시 호

shiho@yonsei.ac.kr

Siemens Simcenter Day 2023

Outline

- **Basics of Quantum Computing**
- **The potential of Quantum Computing in revolutionizing simulation and optimization**
- **Integration of AI, Digital Twin, and Quantum Computing**
  - Quantum advantage
  - Quantum-enhanced and conventional experiments
- **Looking Ahead**

Basics of Quantum Computing

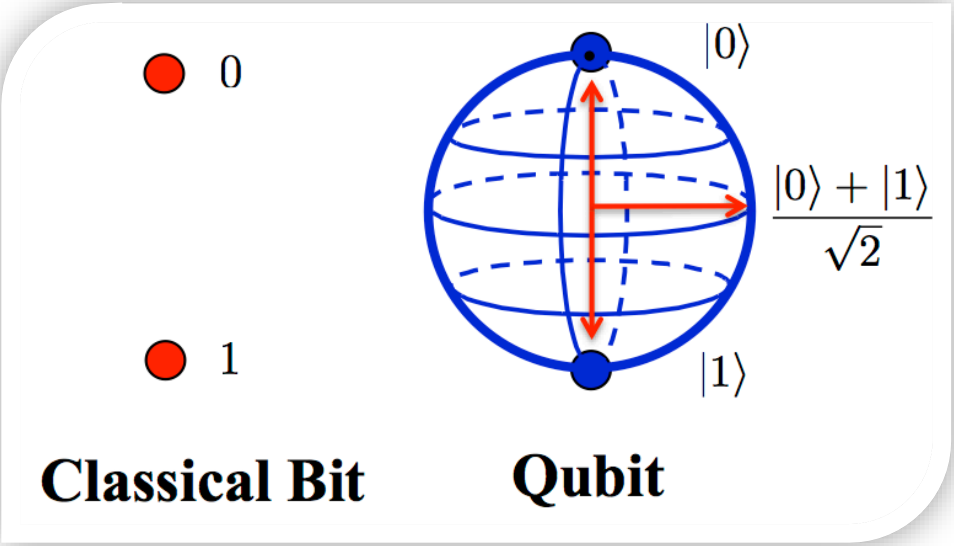
Understanding Quantum Computing without Quantum Physics

- ❖ Quantum (양자) – 영자 역학을 만족하는 물리 상태
- ❖ Qubits (큐빗) : 양자 정보(컴퓨팅)의 기본 단위
- ❖ Superposition (양자 중첩)
- ❖ Entanglement (양자 얽힘)
- ❖ Quantum Coherence (양자 결맞음)
- ❖ Measurement (양자 측정) : 양자 상태 측정하면 양자 상태 붕괴

Basics of Quantum Computing

Understanding Quantum Computing without Quantum Physics

- ❖ Qubits (큐빗) : 양자 정보(커퓨팅)의 기본 단위
- ❖ Superposition (양자 중첩) : |0⟩과 |1⟩ 상태가 중첩

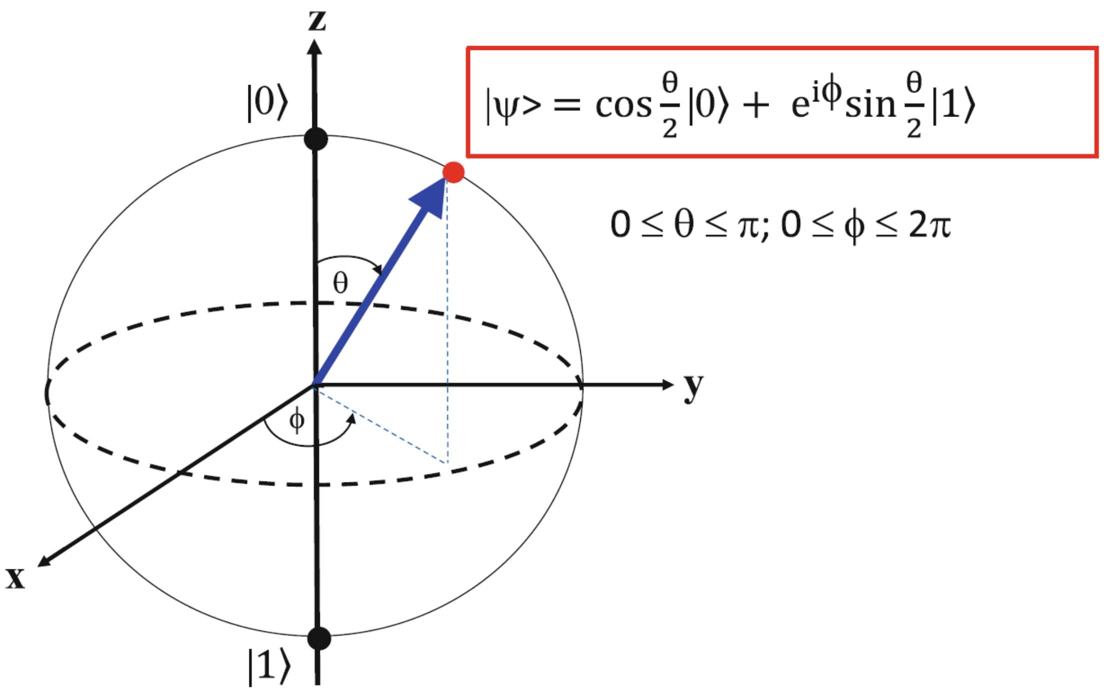


Bloch sphere with |0⟩ and |1 ⟩ at the poles

Basics of Quantum Computing

Understanding Quantum Computing without Quantum Physics

- Qubits (큐빗) : 양자 정보(컴퓨팅)의 기본 단위
- Superposition (양자 중첩)



(single 규빗) 정보의 표현 (중첩 상태)

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

(single qubit) (α, β 는 복소수) 확률 밀도 함수

$$|\alpha|^2 + |\beta|^2 = 1$$

Basics of Quantum Computing

Understanding Quantum Computing without Quantum Physics

- ❖ Qubits (큐빗) : 양자 정보(컴퓨팅)의 기본 단위
- ❖ **Superposition (양자 중첩)**

(two) 큐빗 정보의 표현 (양자 중첩)

$$|\psi\rangle = \alpha_1\alpha_2|0\rangle_1|0\rangle_2 + \alpha_1\beta_2|0\rangle_1|1\rangle_2 + \beta_1\alpha_2|1\rangle_1|0\rangle_2 + \beta_1\beta_2|1\rangle_1|1\rangle_2$$

$$= \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$$

$$\Rightarrow \quad |\psi\rangle = \begin{pmatrix} \alpha_{00} \\ \alpha_{01} \\ \alpha_{10} \\ \alpha_{11} \end{pmatrix}$$

Two 큐빗 중첩 상태
Matrix 표현

확률 밀도 함수 (normalization condition)

$$|\alpha_{00}|^2 + |\alpha_{01}|^2 + |\alpha_{10}|^2 + |\alpha_{11}|^2 = 1$$

Basics of Quantum Computing

Understanding Quantum Computing without Quantum Physics

- Qubits (큐빗) : 양자 정보(커퓨팅)의 기본 소자
- Superpostion (양자 중첩)

(n 규빗) 정보의 표현 (양자 중첩)

$$|\psi\rangle = \sum_{x \in \{0,1\}^n} \alpha_x |x\rangle,\ \alpha_x \in C$$

$$|\psi\rangle = \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_{2^n-1} \end{pmatrix}$$

n 큐빗 중첩 상태
Matrix 표현

(n 규빗) 확률 밀도 함수 (normalization condition)

$$\sum_{x \in \{0,1\}^n} |\alpha_x|^2 = 1$$

Basics of Quantum Computing

Understanding Quantum Computing without Quantum Physics

❖ **Entanglement (양자 얽힘)** : **두 큐빗** 상태가 서로 얽힘

➢ 두 큐빗 상태를 개별 큐빗의 상태로는 표시 불가 $|\psi\rangle \neq |\psi\rangle_1 |\psi\rangle_2$

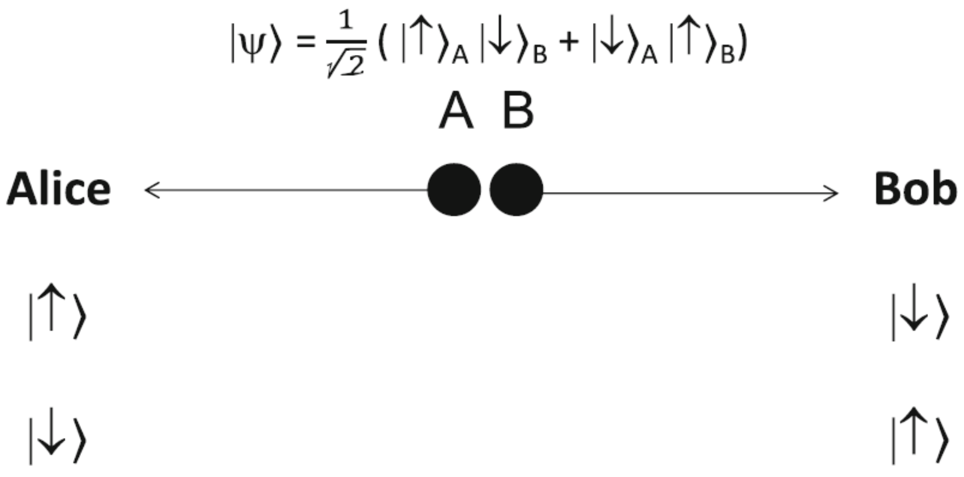
➢ Bell states : 4 entangled two-qubit states

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$$

$$|\Phi^-\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$$

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$



Teleportation of Entangled qubits

Basics of Quantum Computing

Understanding Quantum Computing without Quantum Physics

- **Quantum Coherence (양자 결맞음)** : (Quantum Gates) 양자 컴퓨팅 회로 구현
  - 양자 얽힘이 유지 되는 상태
- **Quantum Gates** : Quantum Operation의 Matrix 표시
  - Single Qubit operations : 단위 큐빗의 위상 변화 (Unitary Transform), 중첩 상태

Quantum operators ($\widehat{U}$) are unitary transformations.

$$\hat{U}|0\rangle = \begin{pmatrix} a & c \\ b & d \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix} = a|0\rangle + b|1\rangle$$

$$\hat{U}|1\rangle = \begin{pmatrix} a & c \\ b & d \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} c \\ d \end{pmatrix} = c|0\rangle + d|1\rangle$$

$$UU^{\dagger} = U^{\dagger}U = I$$

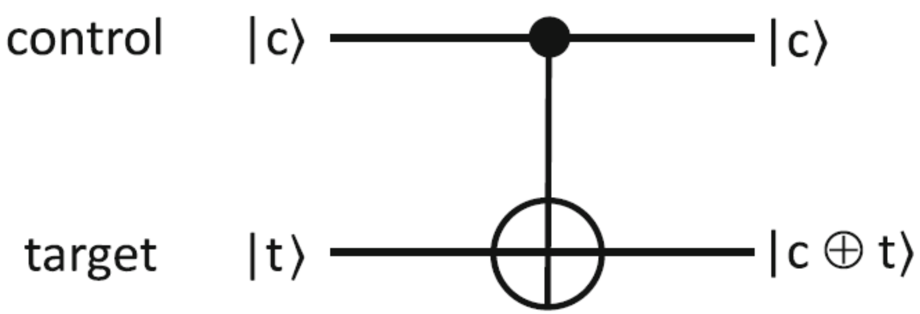
$$U^{-1} = U^{\dagger},$$

Unitary transformations
=> always reversible

Basics of Quantum Computing

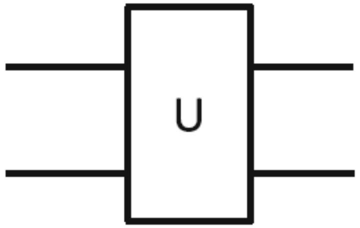
Understanding Quantum Computing without Quantum Physics

❖ Two Qubit Quantum Gates : Control Qubit, Taget Qubit



$$U \begin{pmatrix} \alpha_{00} \\ \alpha_{01} \\ \alpha_{10} \\ \alpha_{11} \end{pmatrix} = \begin{pmatrix} \beta_{00} \\ \beta_{01} \\ \beta_{10} \\ \beta_{11} \end{pmatrix}$$

$|\psi_i\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$



$|\psi_f\rangle = \beta_{00}|00\rangle + \beta_{01}|01\rangle + \beta_{10}|10\rangle + \beta_{11}|11\rangle$

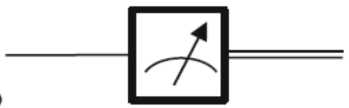
Basics of Quantum Computing

Understanding Quantum Computing without Quantum Physics

❖ Measurement (측정) :

quantum state

$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$



classical state

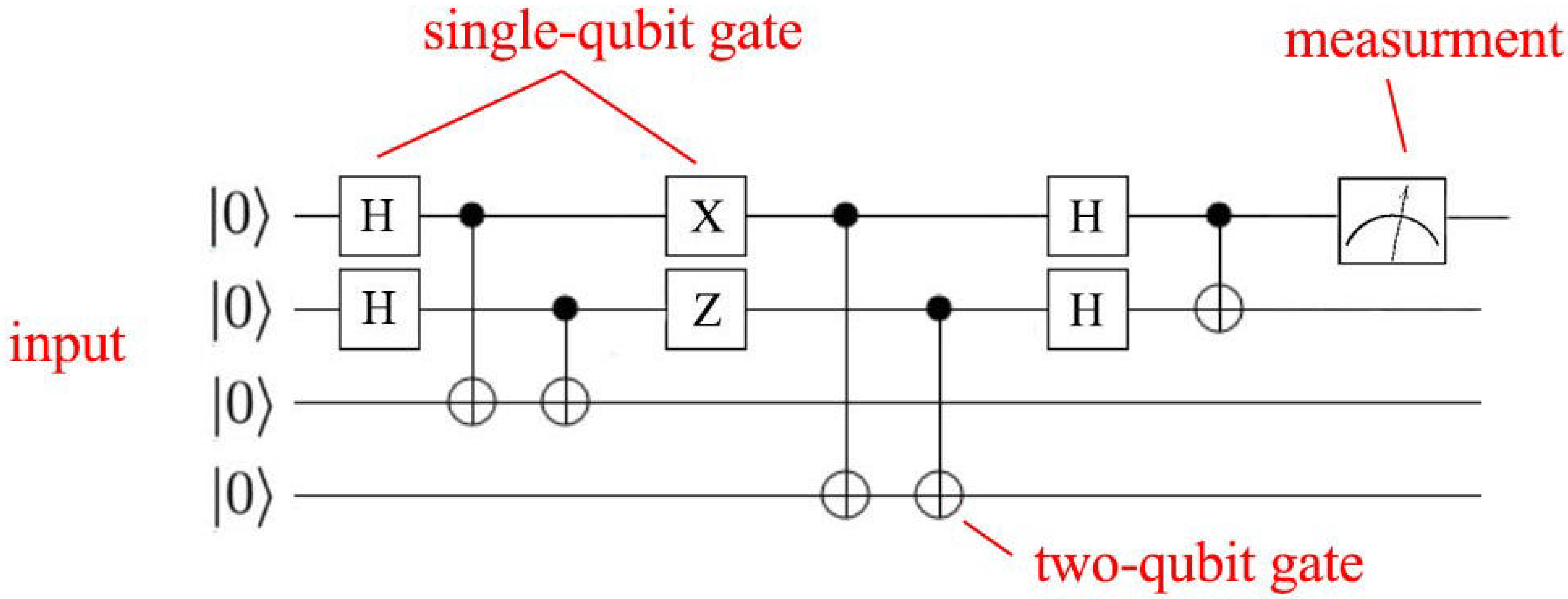
$|0\rangle$ or $|1\rangle$

측정하면 양자 상태의 붕괴 :

Basics of Quantum Computing

Understanding Quantum Computing without Quantum Physics

❖ (Example) Programming with Quantum Gates



Basics of Quantum Computing

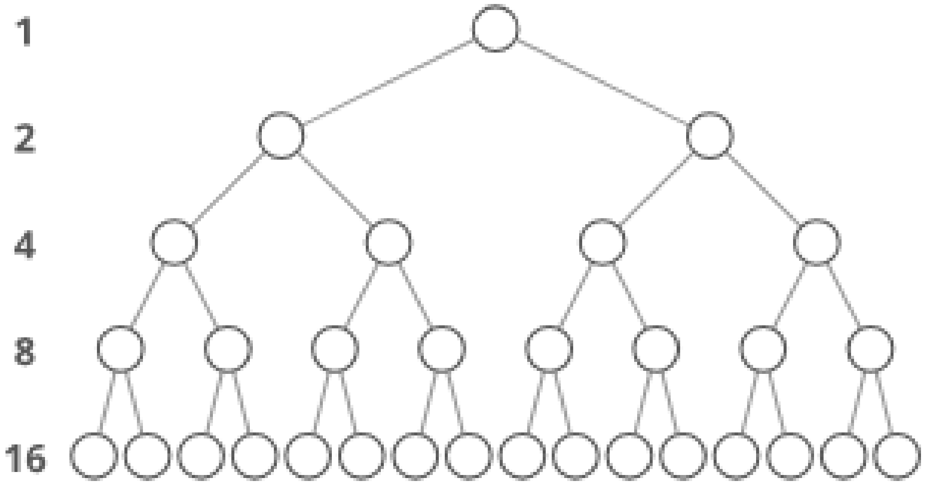
양자 중첩 이용 : 양자 병렬성 :

- **지수함수(Exponential)의 복잡도 $\mathcal{O}(k^n)$**

  => 다항 함수(polynomial) 복잡도 $\mathcal{O}(n^k)$

Binary tree

n states N (2^n)



Sequential 2^n states search

Classic bits (2^n)

0,1

00, 01, 10, 11

000, 001, 010, 011… 111

0000, 0001, ……………1111

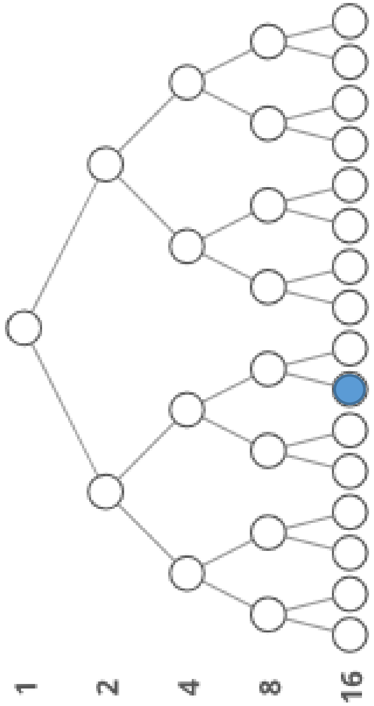
n Qubits

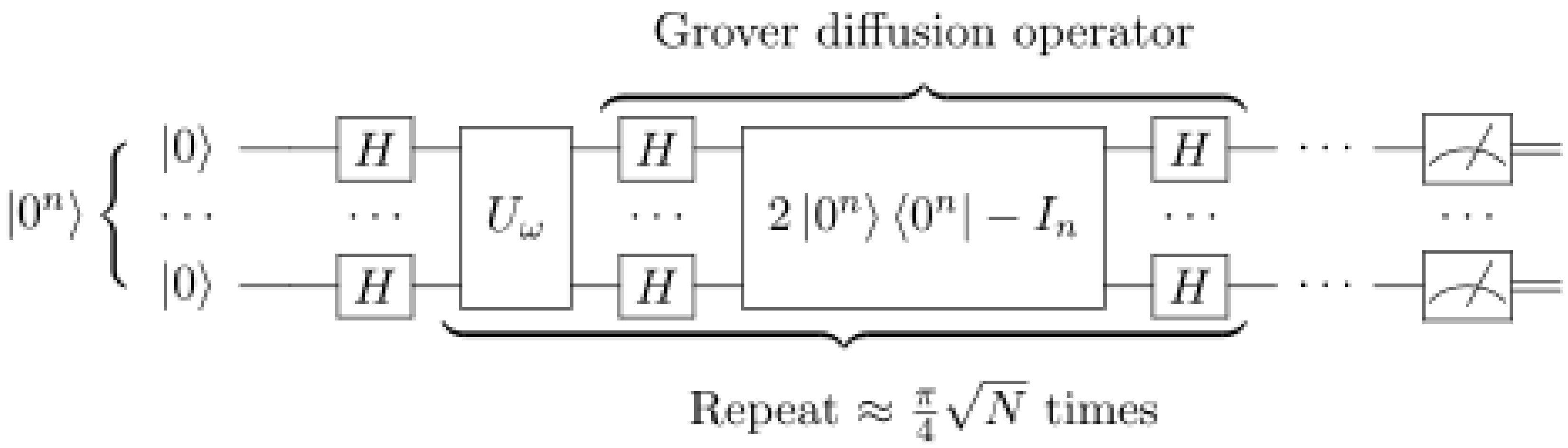
Superposition of 2^n states

Basics of Quantum Computing

Search Algorithm Example :

양자 중첩 이용 : Grover's search algorithm ; $\mathcal{O}(\sqrt{N})$





Classic Sequential search : $\mathcal{O}(N)$

Basics of Quantum Computing

Example: Classic vs. Quantum Computing algorithms

문제 1 : $z = f\ (x, y) = (x + y)$ (ex : if x=3, y=5 then z=8)

문제 2 : $\{x, y\} = f^{-1}(z)$ (ex : Find x, y which satisfying z=8)

Classic Computer : x, y가 64-bit 인 경우
문제1 : 쉽게 해결
문제2 : 2^n * 2^n = 16T * 16T = 256*10^{24} = 256 Yotta iterations problem
(100 TOPs GPU 적용시 2.56*10^{12} sec ≅ 1.2*10^{7} Hour ≅ 1350 Years)

Quantum Computer : x, y가 64-bit 인 경우
문제2: n+n=64+64 = 126 Qubits search problem
(~ 수분 이내에 해결 가능)

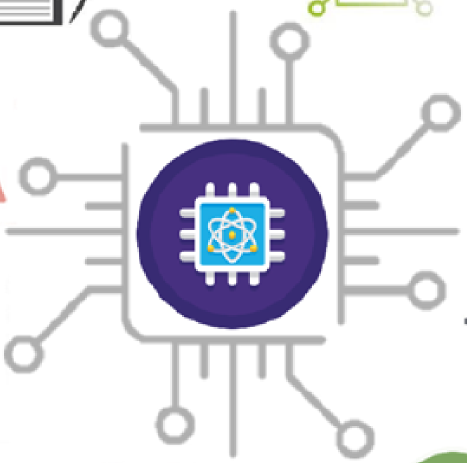
The potential of Quantum Computing in revolutionizing simulation and optimization

양자 컴퓨팅 활용 기대 분야

IT·AI·데이터 과학 : 머신 러닝의 위한 고속 클러스터링, 이미지 인식 고속 학습, 데이터베이스 탐색, 역행렬 계산, 양자기계학습

보안 : 소인수분해(암호 해독), 양자네트워크, 양자 클라우드 계산, 양자머니, 양자인증

의료 : 암 치료용 약물 발견/최적 복용량 산출, 개인 맞춤형 의료의 고속화
제약 : 단백질의 3차원 구조 최적화/분석 (알츠하이머병 등의 특효약 개발)



화학·재료 : 분자설계최적화, 양자화학 계산, 전지와 촉매의 최적화, 화학반응 탐색, 화학반응의 양자역학적 시뮬레이션

항공우주 : 유체역학적으로 최적화된 기체 설계, 비행 제어 시스템의 버그 잡기 최적화

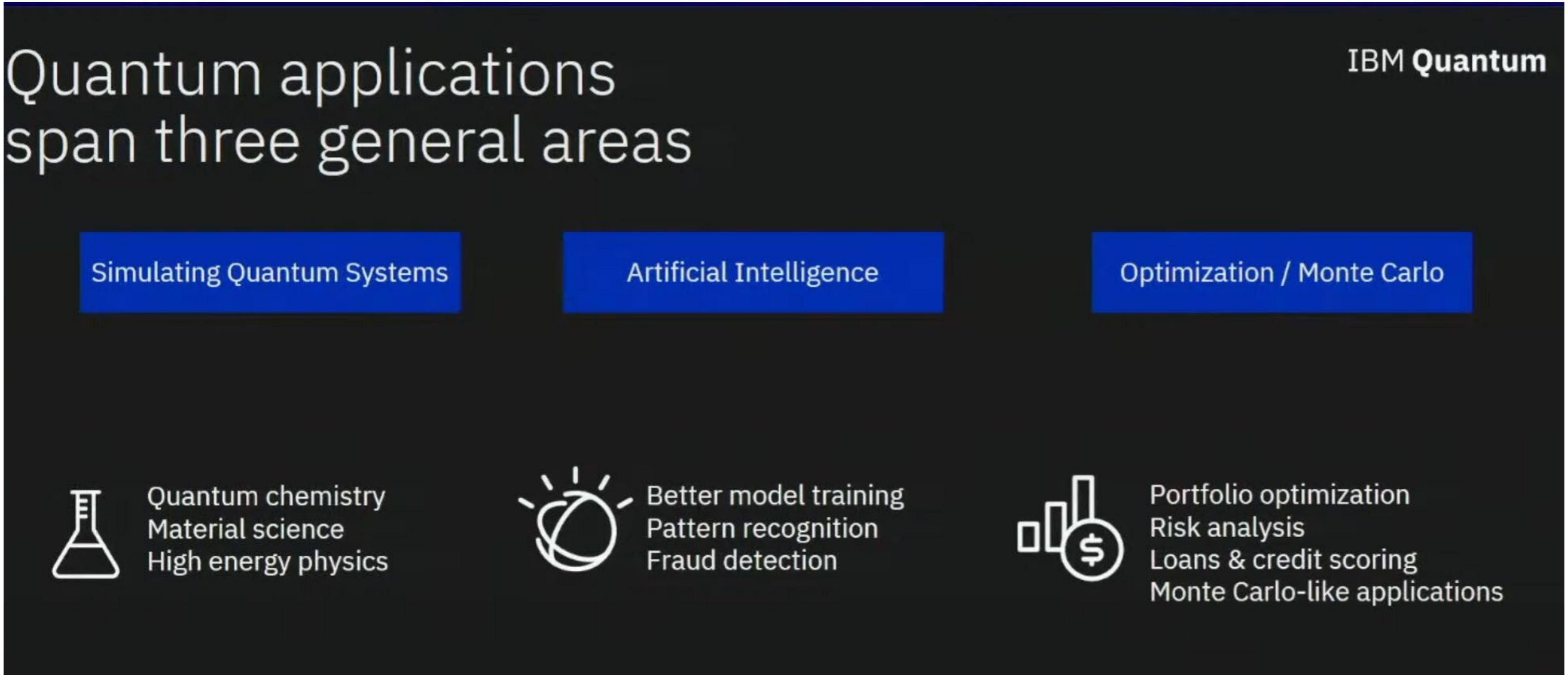
과학 기술 프론티어 : 신기한 물성 탐색, 고온 초온도, 기초 물리, 블랙홀

물류 : 비행기, 선박, 트럭 등의 물류 최적화
자동차 : 도시 교통 서비스 최적화

금융 : 포트폴리오 최적화, 리스크 관리, 옵션 가격 결정

양자정보기술백서, 미래양자융합포럼, 과기정통부 2022

The potential of Quantum Computing in revolutionizing simulation and optimization



IBM Quantum 2022

The potential of Quantum Computing in revolutionizing simulation and optimization

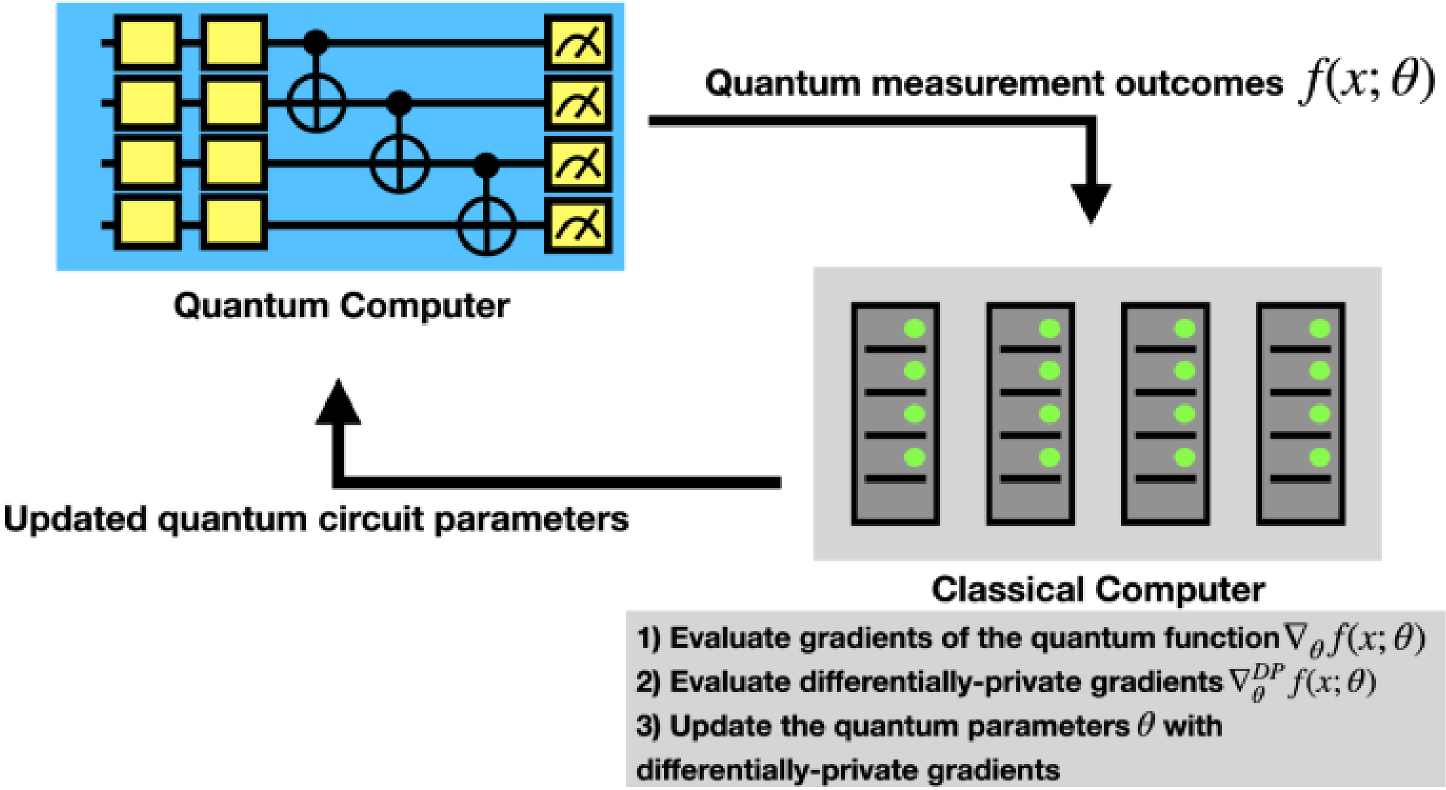
	Chemicals and Petroleum	Distribution and Logistics	Financial Services	Health Care and Life Sciences	Manufacturing
● Chemical Simulation	Chemical product design Surfactants, Catalysts			Drug Discovery Protein Structure Predictions	Materials Discovery Quantum Chemistry
■ Scenario Simulation		Disruption Management	Derivatives Pricing Investment Risk Analysis	Disease Risk Predictions	
▲ Optimization	Feedstock To Product Oil Shipping / Trucking Refining Processes	Distribution Supply Chain Network Optimization Vehicle Routing	Portfolio Management Transaction Settlement	Medical/Drug Supply Chain	Fabrication Optimization Manufacturing Supply Chain Process Planning
◆ AI/ML	Drilling Locations Seismic imaging	Consumer Offer Recommender Freight Forecasting Irregular Behaviors (ops)	Finance Offer Recommender Credit/Asset Scoring Irregular Behaviors (fraud)	Accelerated Diagnosis Genomic Analysis Clinical Trial Enhancements	Quality Control Structural Design & Fluid Dynamics

IBM Quantum 2022

Integration of AI, Digital Twin, and Quantum Computing

Hybrid quantum-classical framework

- Interfacing classical optimization algorithms with VQC-based QML algorithms
- The quantum circuit parameters are updated and fed back to the quantum computer.



Watkins, W.M., et.al, Quantum machine learning with differential privacy. Sci Rep 13, 2453 (2023)

Integration of AI, Digital Twin, and Quantum Computing

Quantum machine learning Researches

Long-term: Quantum Linear Algebra

Exponential or polynomial speed-up in

- Support vector machine
- Principle component analysis
- Bayesian methods
- ...

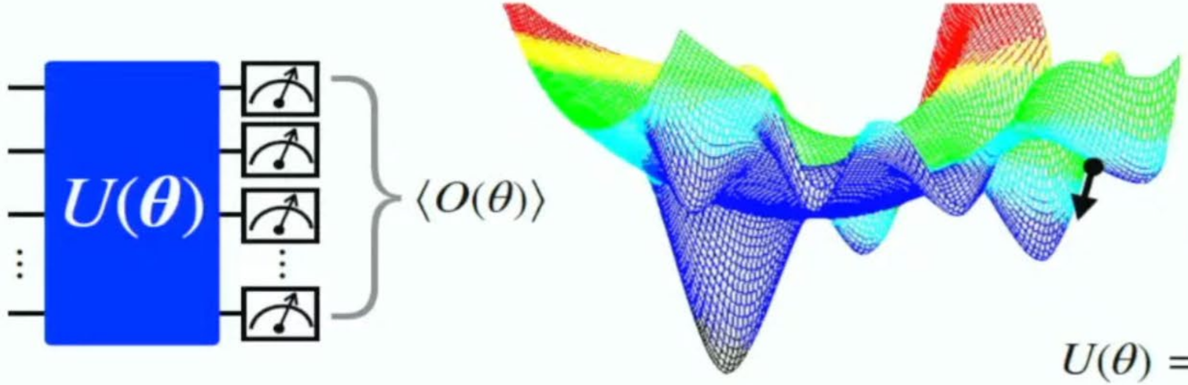
Near-term QML

- Kernel method
- Variational (trainable) Quantum Circuits
- (Non-adiabatic) Quantum annealing
- Quantum-inspired classical algorithms

* Constant factor analysis beyond big-O analysis is important.

Integration of AI, Digital Twin, and Quantum Computing

Vibrational Quantum Circuits



$$L(\theta) = f\left(\langle O(\theta)\rangle\right)$$

$$\langle O(\theta)\rangle = \mathrm{Tr}\left(OU(\theta)\rho U^{\dagger}(\theta)\right)$$

$$U(\theta) = \exp\left[-i\theta P/2\right], P \in \{I, \sigma_x, \sigma_y, \sigma_z\}^{\otimes n}$$

$$\frac{\partial\langle O(\theta)\rangle}{\partial\theta} = \frac{1}{2}\left\{\mathrm{Tr}\left(OU\left(\frac{\pi}{2}\right)U(\theta)\rho U^{\dagger}(\theta)U^{\dagger}\left(\frac{\pi}{2}\right)\right) - \mathrm{Tr}\left(OU\left(-\frac{\pi}{2}\right)U(\theta)\rho U^{\dagger}(\theta)U^{\dagger}\left(\frac{-\pi}{2}\right)\right)\right\}$$

→ Analytical gradient can be calculated with two measurements!

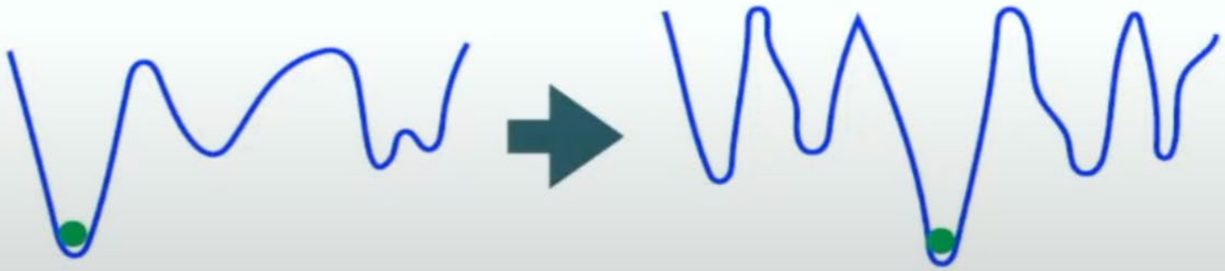
Integration of AI, Digital Twin, and Quantum Computing

Adiabatic Quantum computing

$$i\frac{d|\psi(t)\rangle}{dt} = H(t)|\psi(t)\rangle \qquad H(t)|\epsilon_j(t)\rangle = \epsilon_j(t)|\epsilon_j(t)\rangle,\ \ \epsilon_j(t) \le \epsilon_{j+1}(t)\ \forall\, j \in \{0,\ldots,\dim(H)-1\}$$

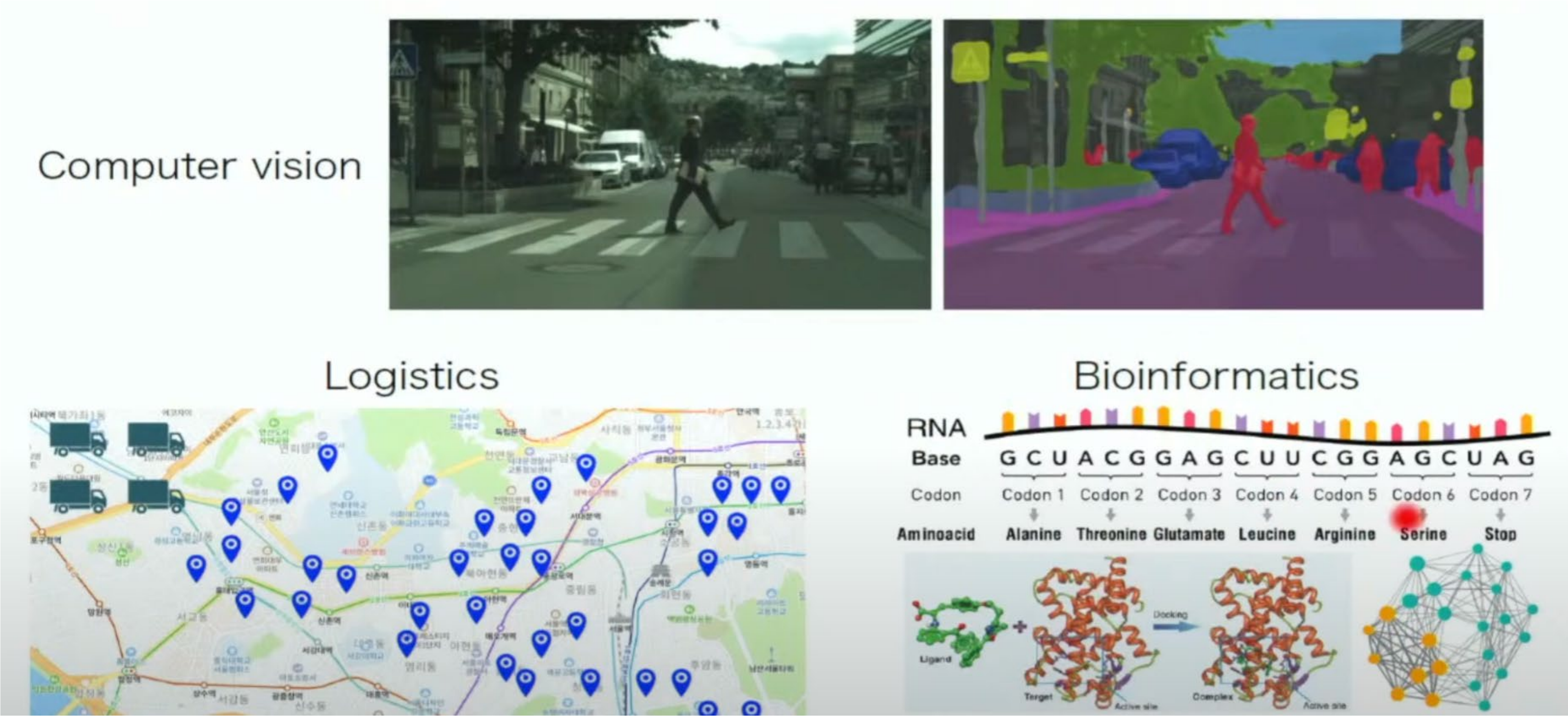
- Adiabatic theorem:
  $|\epsilon_j(0)\rangle$ will remain in $|\epsilon_j(s)\rangle$ for all $s \in [0,1]$ where $s = t/T$ if $T \gg O(|\epsilon_j - \epsilon_k|^{-2})$, $k \neq j$

$$H(t) = \left(1 - \frac{t}{T}\right) H_B + \frac{t}{T} H_P$$



Integration of AI, Digital Twin, and Quantum Computing

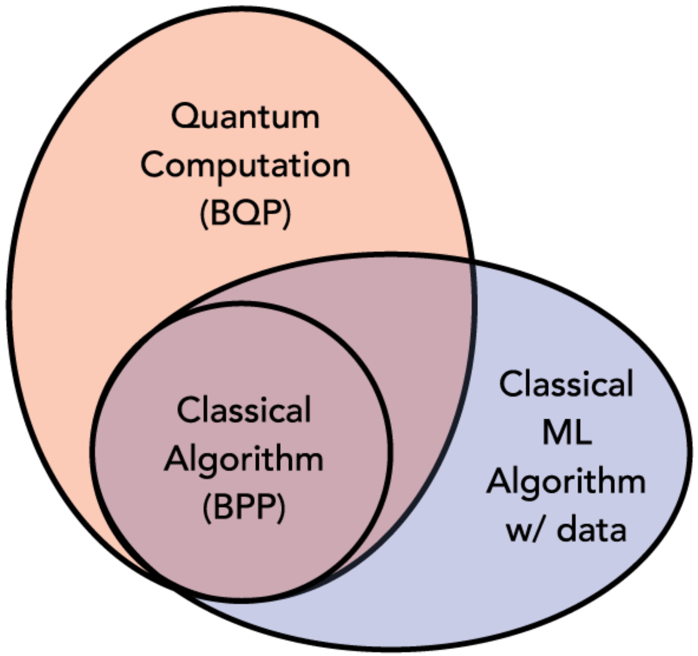
Ising Hamiltonian – Combinational Optimization

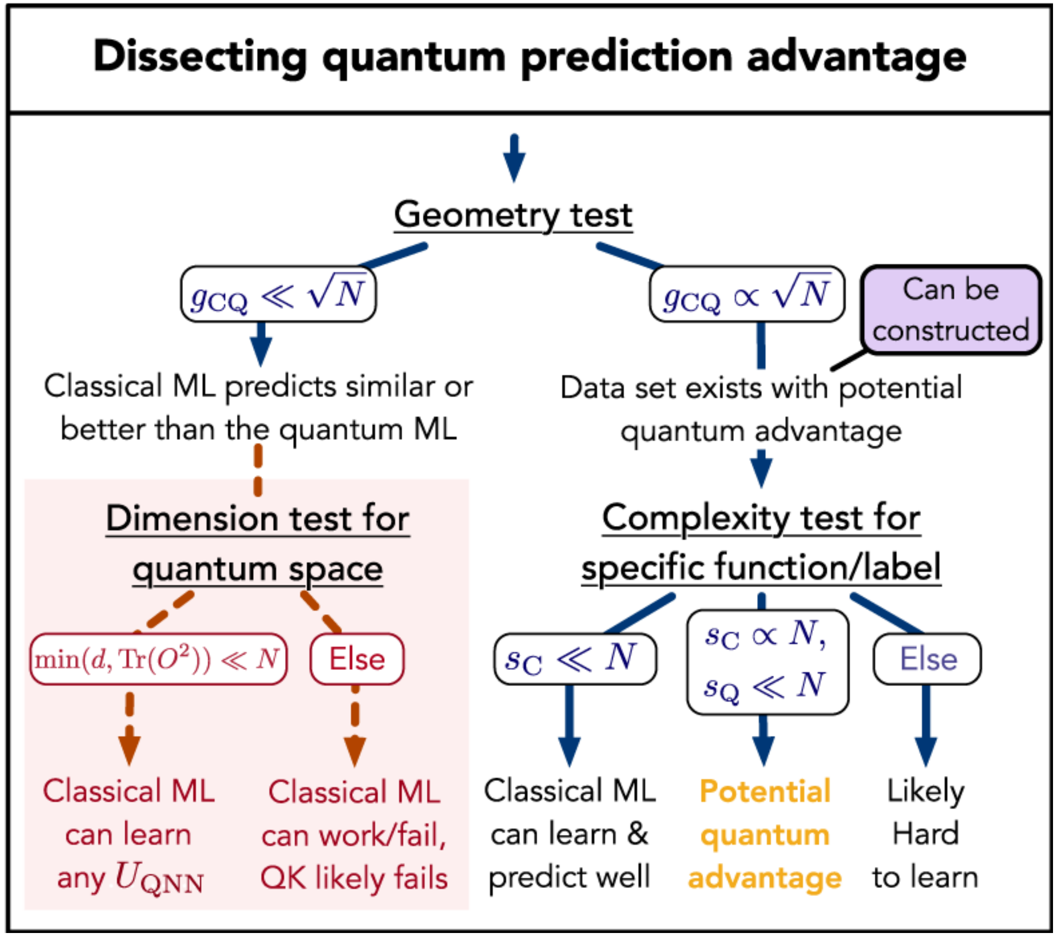


QML model advantages (1. Less data)

Measure of an advantageous quantum/classical prediction

Model complexities (s_C , s_Q), *and* geometric quantity g_{CQ}



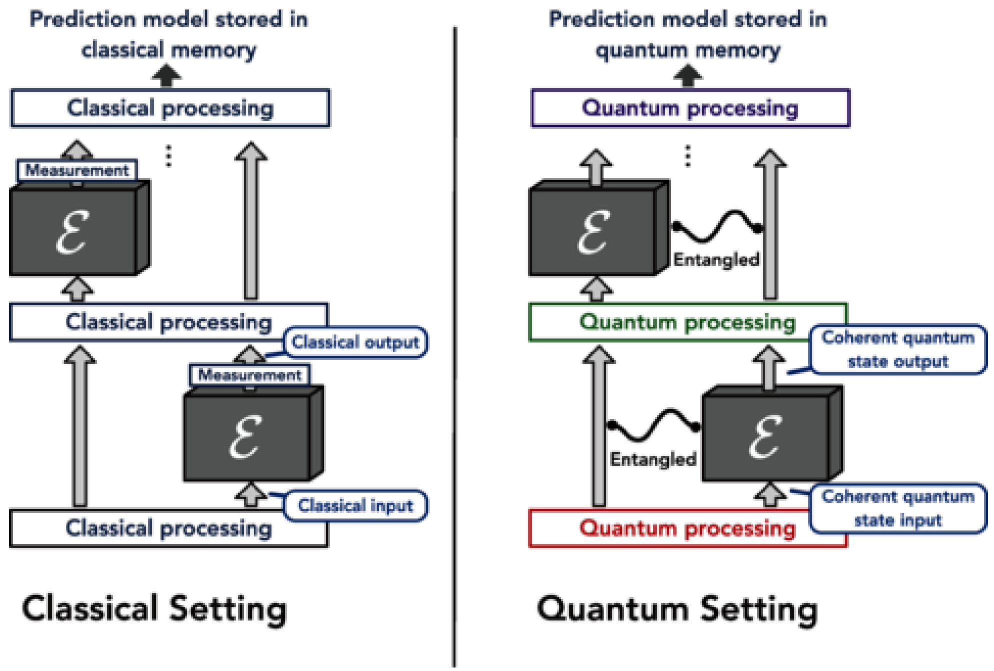


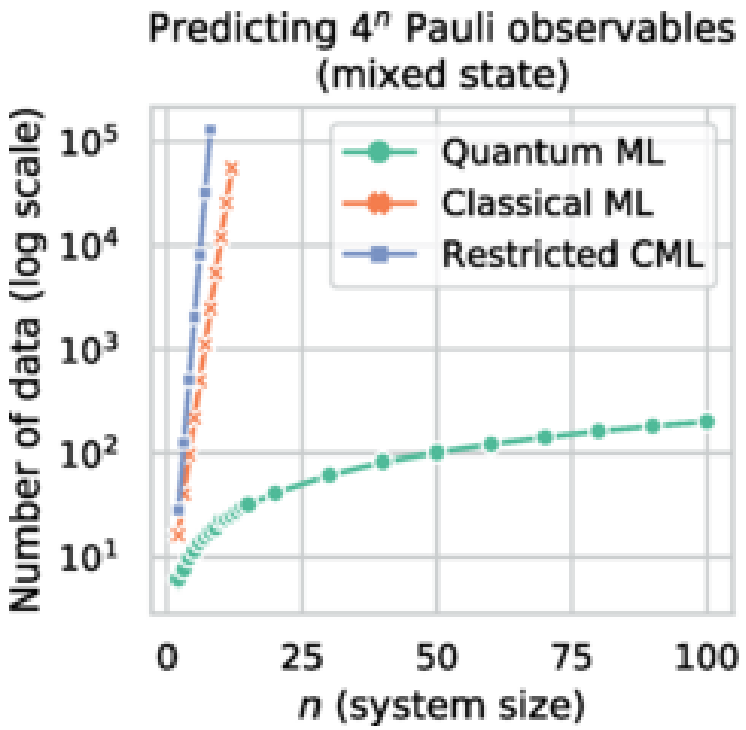
Huang, HY. , et al. Power of data in quantum machine learning. Nat Commun 12, 2631 (2021)

QML model advantages (1. Less data)

Generalization performance of quantum phase recognition

This experimental work demonstrated **exponential advantage** in quantum machine learning





Hsin-Yuan Huang, et.al, Phys. Rev. Lett. **126**, (2021)

QML model advantages (2. Less parameters)

Generalization in quantum machine learning from few training data

- **Theoretical bounds on the generalization error** in vibrational QML bounded by $\sqrt{T/N}$ (trainable gates T, number *N* of training data)

- To obtain good generalization for an efficiently implementable QML model, Only requires $T \in \mathcal{O}(poly\, n)$ and efficient amount of training data, $N \in \mathcal{O}(poly\, n)$

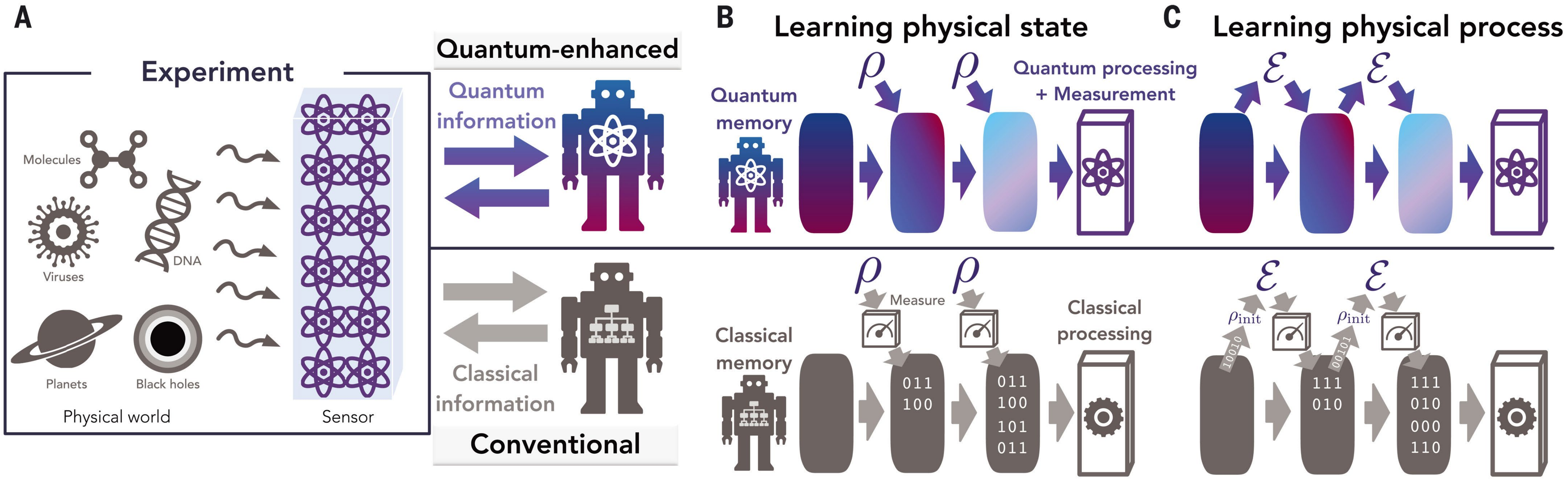
- QCNNs have only $T = \mathcal{O}(log\, n)$ parameters, and QCNNs have good generalization error for quantum phase recognition with **only poly logarithmic training resources**, $N \in \mathcal{O}(log^2\, n)$

Poly logarithmic function in *n* is a polynomial in the logarithm of *n*, $(\log n)^k$,

Matthias C. Caro, et. al, Nature Communications, 13, 4919 (2022)

Quantum-enhanced and conventional experiments

Illustration of quantum-enhanced and conventional experiments.



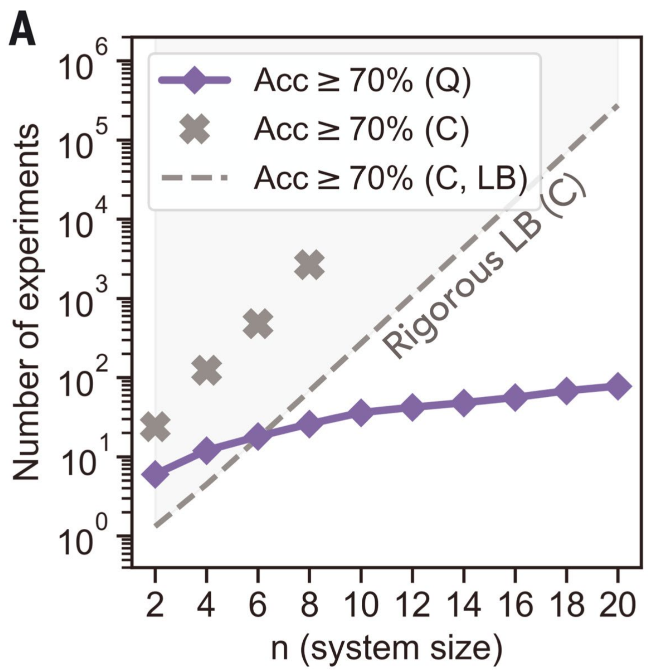
Quantum advantage in learning from experiments, SCIENCE, Vol 376, Issue 6598, Jun 2022

Quantum advantage in learning from experiments

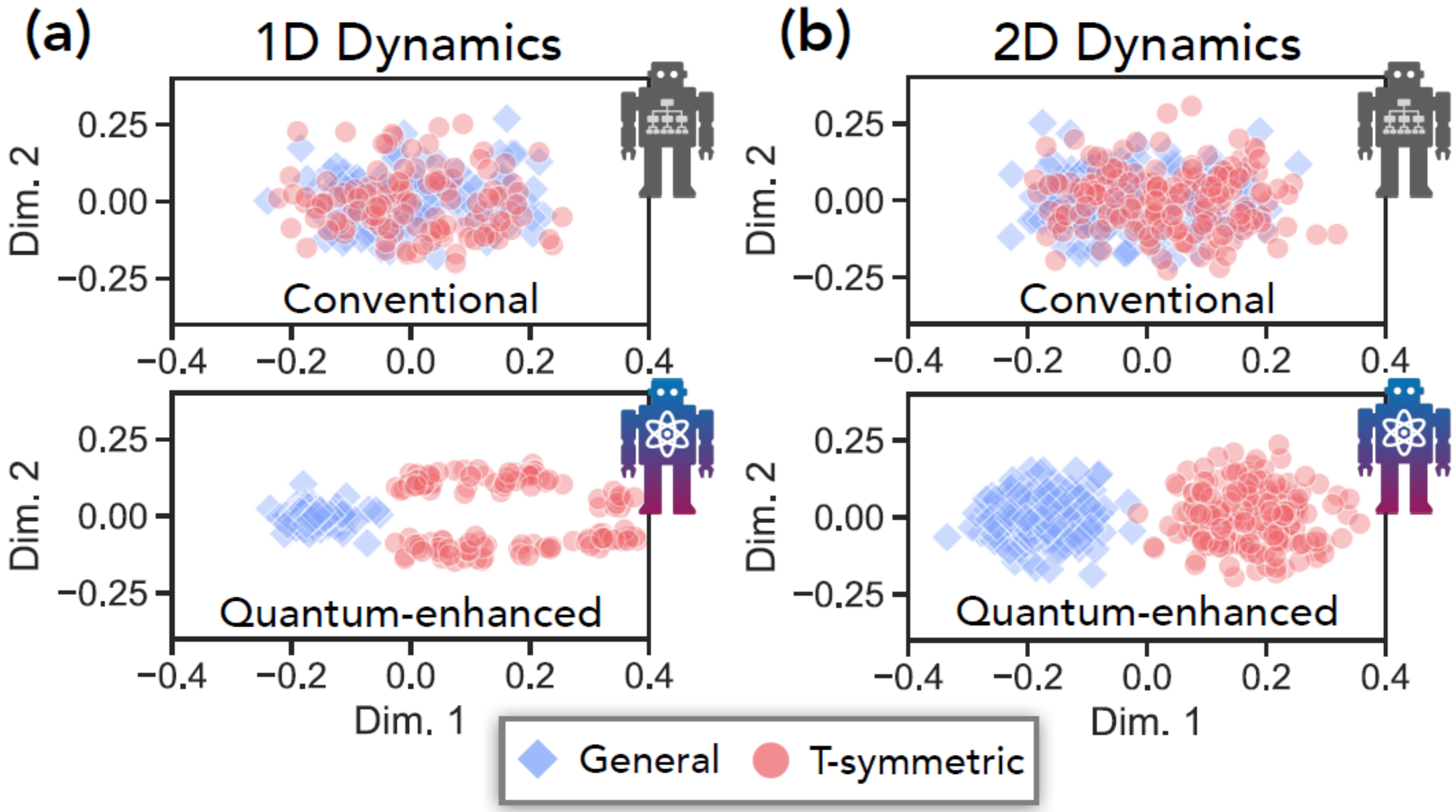
Demonstrations of quantum advantage.

Quantum advantage in learning physical states.

(4. Less iterations)

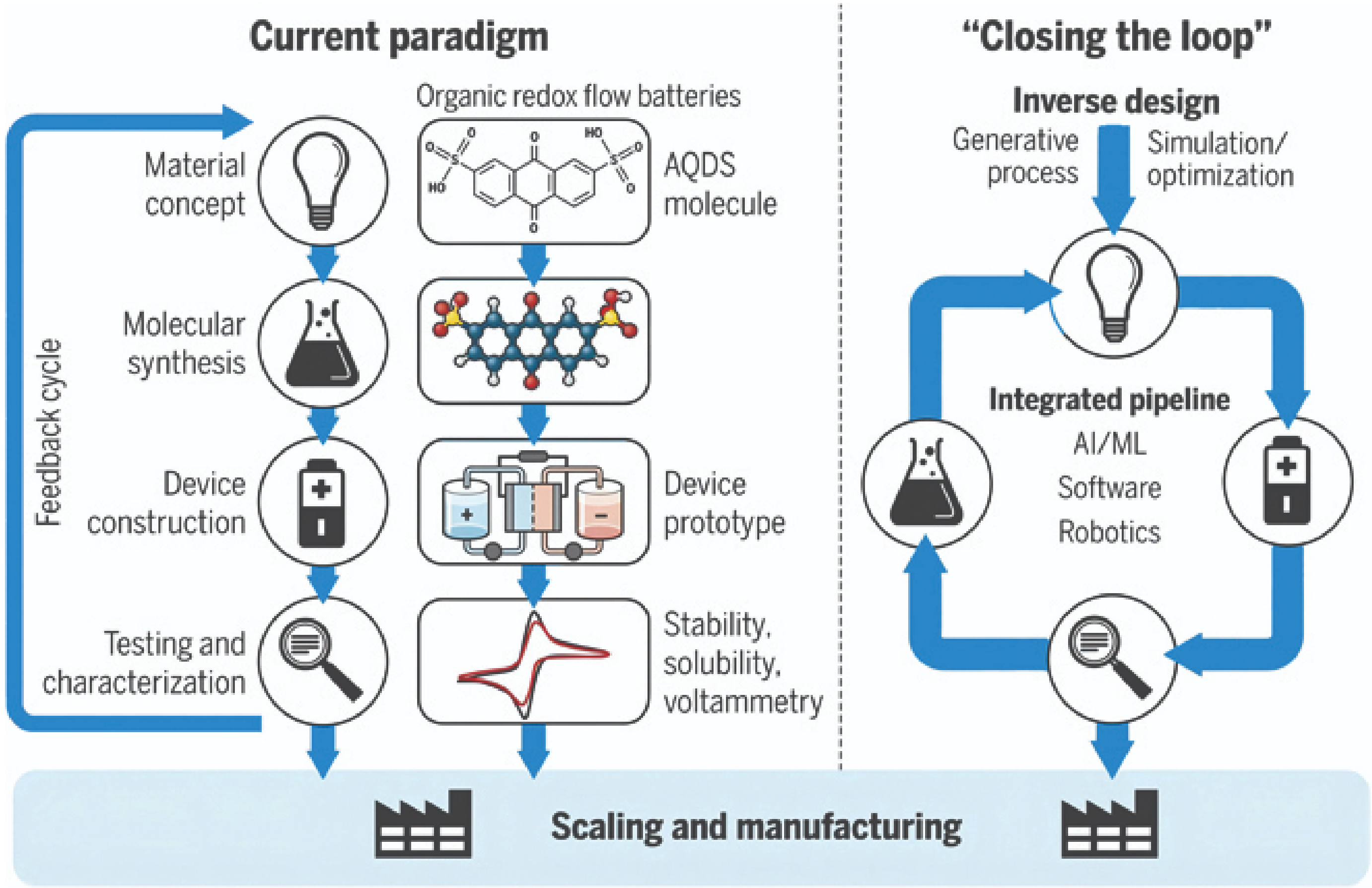


(3. Less experiments)



Quantum advantage in learning from experiments, SCIENCE, Vol 376, Issue 6598, Jun 2022

Looking Ahead
Challenges and opportunities in quantum processing



(Inverse Design)

Intelligent Computing: The Latest Advances, Challenges, and Future, DOI: 10.34133/icomputing.0006

Looking Ahead

- ❖ 현재는 NISQ (Noise Intermediate Scale Quantum) 시대
- ❖ **Quantum Advantage가 보이지만 본격적인 QC 활용을 위해서는 FT(Fault Tolerant) QC, 최소 10K Qubits 필요**
- ❖ 2030년 초반에 FTQC 시대가 본격 도래될 것으로 전망

Summary

❖ Quantum advantage :

- 1) less data, 2) less iterations, 3) less parameters, 4) less experiments,
- 알고리듬을 잘 설계하면 지수함수적인 양자 이득 구현 가능.

❖ 현재의 Classic HPC로는 해결할 수 없는 문제들 해결 가능

❖ **Quantum Leap : Harnessing Artificial Intelligence, Digital Twin Technology, and Quantum Computing for Next-Generation Simulation and Optimization**

- Simulation, optimization, Machine Learning, AI
- Inverse design : 새로운 개발 방법, 모든 변수의 가능성 고려