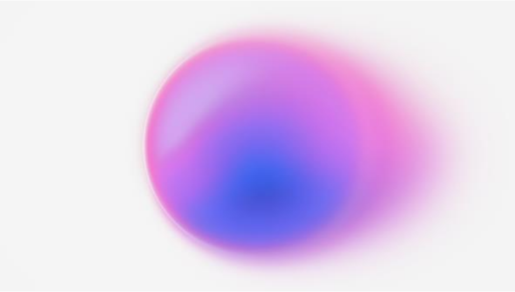
Quantum Algorithms for Biomedical and Translational Applications

Aritra Bose, PhD
Filippo Utro, PhD

IBM Quantum
IBM T. J. Watson Research Center, New York, USA

What is Quantum Computing?

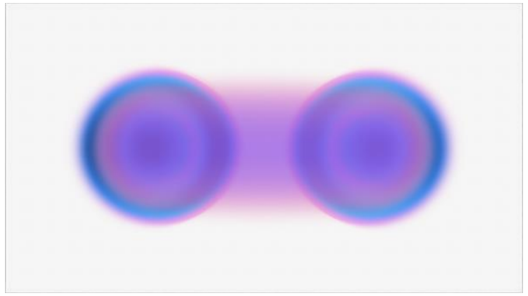
Computer that exploits quantum mechanical properties to process information



- Superposition
- A quantum system existing in multiple states simultaneously until it is measured

↓

Parallelism



- Entanglement
- Information shared jointly between entangled pairs or groups

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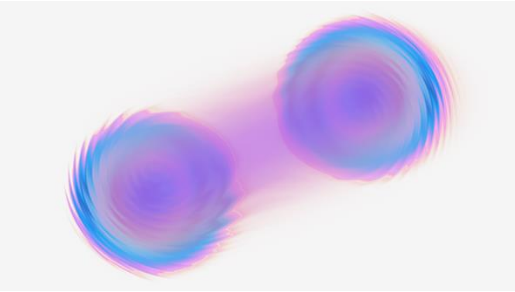
Correlation



- Interference
- Interaction that affects likelihood of solutions

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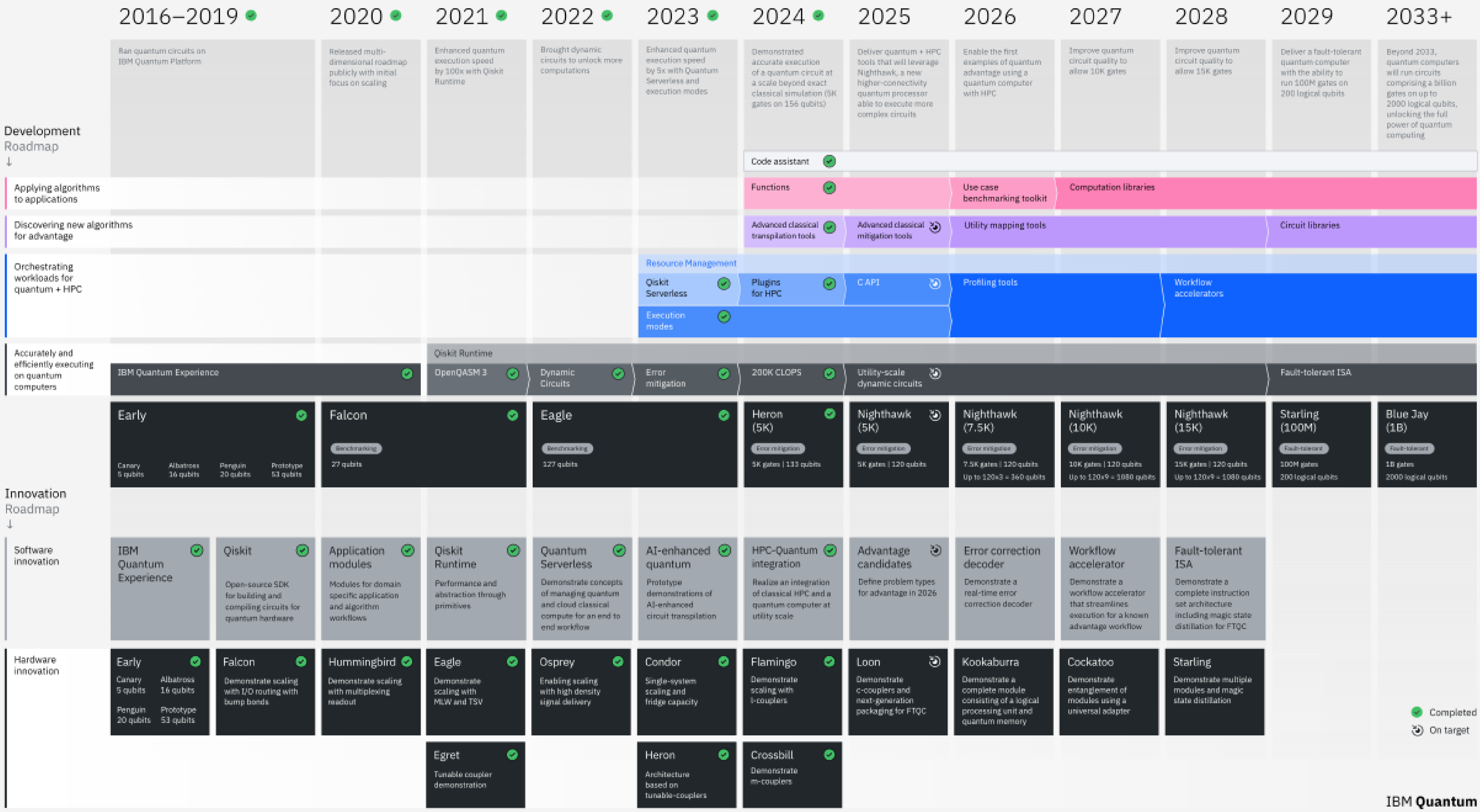
Convergence

IBM Quantum: System Two (Utility Scale)

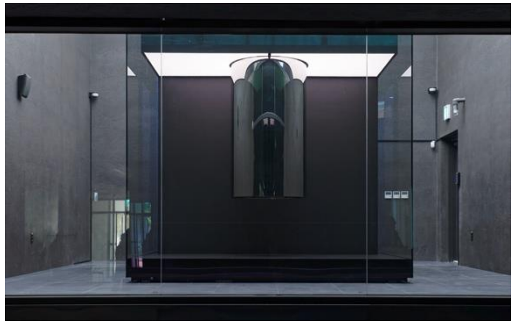
Development Roadmap



IBM has deployed 75+ systems since 2016.

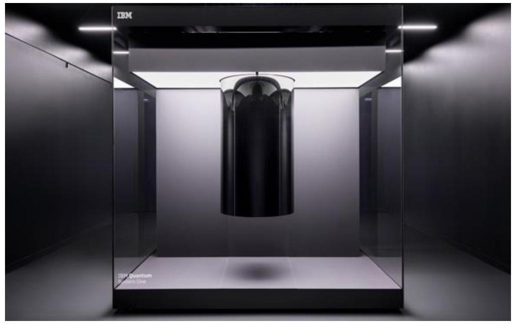
Today, there are 13 utility-scale quantum computers (133+ qubits) operational in Poughkeepsie, NY; our European data center; and in client locations around the world.

Discovery Accelerator - Cleveland Clinic
Ohio, USA
March 2023



Quantum Computational Center - Yonsei University - Seoul, South Korea
September 2024

Quantum Computational Center University of Tokyo
Shin-Kawasaki, Japan June 2021



Discovery Accelerator - PINQ [2]
Bromont, Canada
September 2023

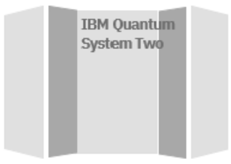
Quantum Computational Center Rensselaer Polytechnic
Troy, New York
April 2024

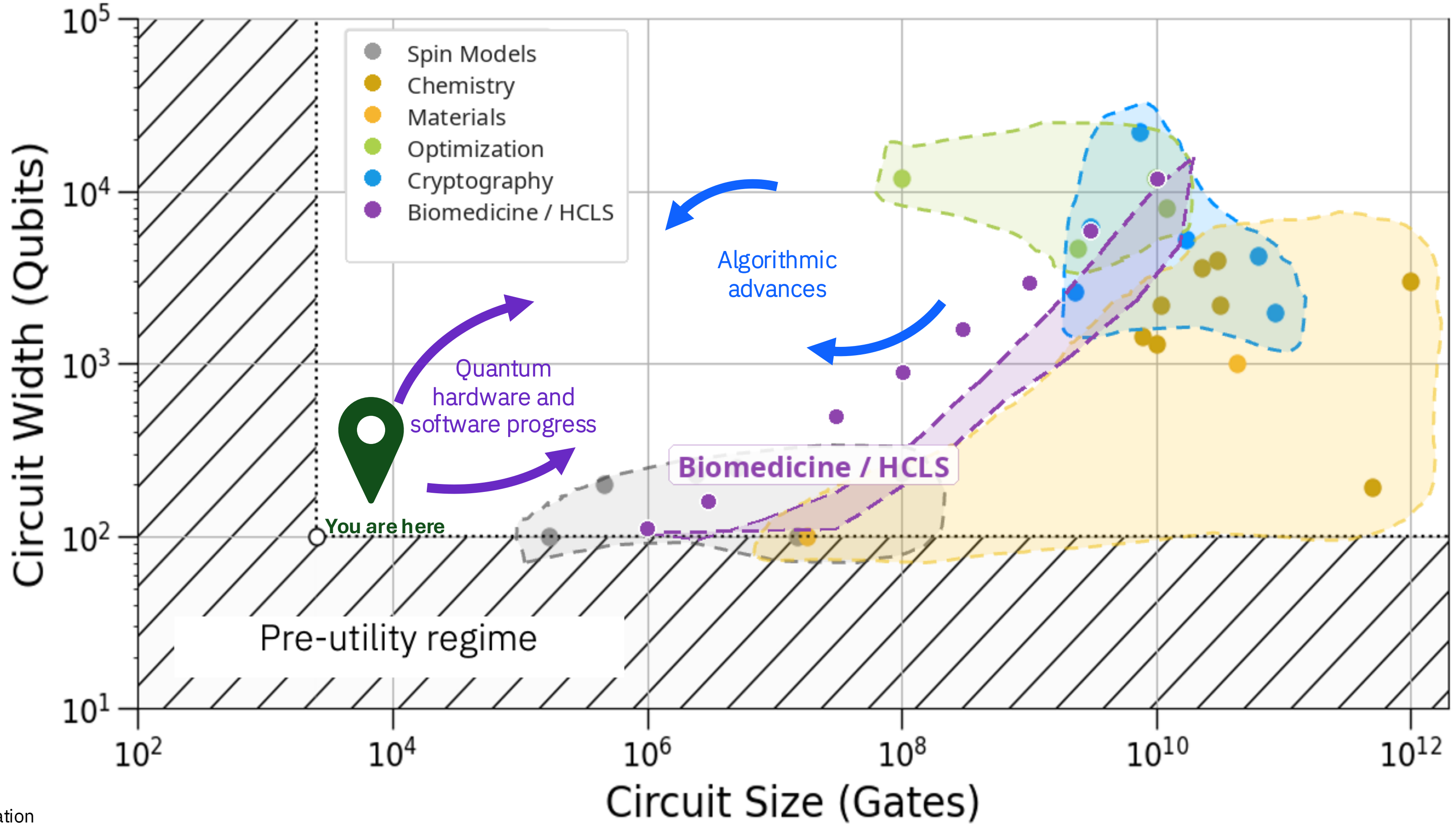
JHPC-quantum - Riken
Kobe, Japan, May 2025

IBM-Euskadi Quantum Computational Center, BasQ
San Sebastián, Spain, May 2025

National Quantum Algorithm Center
Chicago, USA. Projected September 2025

Useful Quantum = Hardware + Algorithm + Applications





The computationally complex problems exist across almost every industry

Banking
- Fraud monitoring
- Portfolio optimization
- Risk simulation
- Customer analytics
- Time series forecasting

Automotive
- Battery material design
- Material design
- Mobility as a Service
- Quality control
- Self-driving and ADAS
- Production optimization

Chemicals
- Sustainable products
- Low-carbon manufacturing
- Resilient supply chains
- Process optimization
- Asset health

Life sciences
- Efficient drug research and development
- Clinical trials
- Tractable protein folding
- Call-centric therapeutics
- mRNA

Healthcare
- Accelerated diagnoses
- Personalized interventions
- Adherence to drugs
- Biomarkers
- Image processing

Logistics
- Global logistics optimization
- Disruption management
- Routing optimization
- Predictive maintenance
- Forecasting

Public services
- Security/safety
- Multimodal transport
- City resource planning
- Disaster management
- Fraud detection in tax and social

Insurance
- Catastrophe modeling
- Precise customer profiling
- Efficient risk management
- Optimized pricing of premiums

Electronics
- Faster product design
- Circuit defect identification
- Process optimization
- Production optimization
- Quality control

Airlines
- Forecasting and revenue
- Irregular operations
- Network planning
- Safety and maintenance
- Hyper-personalization

Energy and utilities
- Energy trading
- Optimization of energy grid
- Renewables system design
- Energy forecasting
- Hyper-personalization
- Asset health

Aerospace
- Material discovery
- Aircraft design
- Asset health
- Corrosion and material interaction
- Fuel efficiency

Oil and gas
- Emissions reduction
- Reservoir simulation
- Virtual flow meters
- Subsurface modeling
- Failure prediction

Telecom
- Network optimization
- Network anomaly detection
- Contextual customer segmentation
- Cybersecurity network

Perspectives on Quantum Algorithms for Healthcare and Life Sciences

JCTC Journal of Chemical Theory and Computation
Open Access

pubs.acs.org/JCTC
Perspective

A Perspective on Protein Structure Prediction Using Quantum Computers

CellPress OPEN ACCESS
Trends in Pharmacological Sciences
Opinion

How can quantum computing be applied in clinical trial design and optimization?

Patterns
CellPress OPEN ACCESS
Perspective

How quantum computing can enhance biomarker discovery

npj | digital medicine
Article
Published in partnership with Seoul National University Bundang Hospital
https://doi.org/10.1038/s41746-025-01597-z

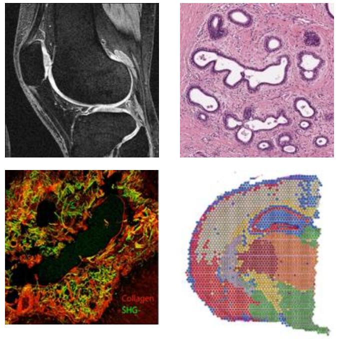
A systematic review of quantum machine learning for digital health

nature reviews molecular cell biology
https://doi.org/10.1038/s41580-025-00918-0
Roadmap
Check for updates

Advancing single-cell omics and cell-based therapeutics with quantum computing

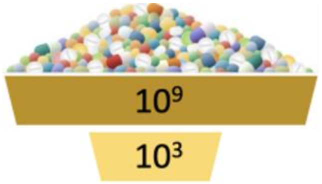
An Ecosystem of Quantum Algorithms for Healthcare and Life Sciences

Biomedical Imaging



- MRI denoising, super-resolution, segmentation, etc.
- X-ray/DXA scans
- Histopathology
- Second-Harmonic Generation

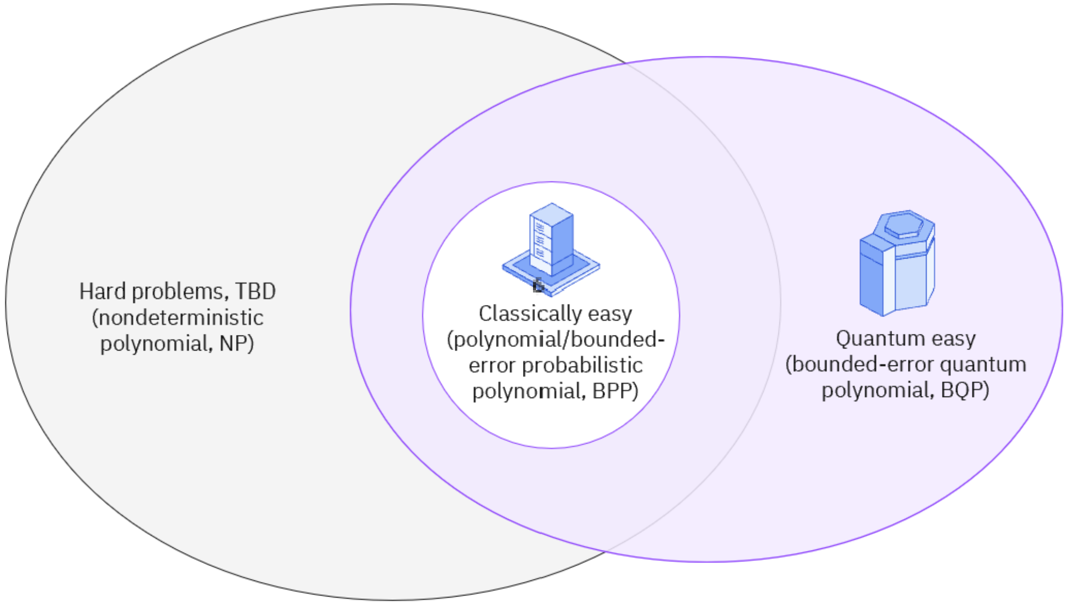
Virtual Screening



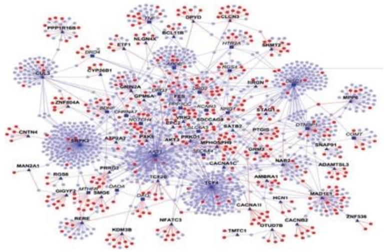
- Conformational Space Search
- Binding Affinity Prediction
- Post-Translational Modification
- Limited Experimental Data in ADMET

Cancer Immunotherapy

- Find potential signaling domains
- Accurately predict immunogenicity/cytoxicity.

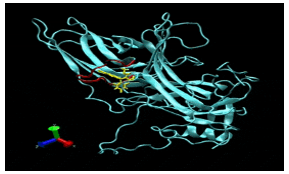


Network Biology



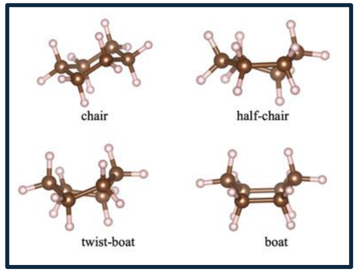
- Modeling Cellular Networks & Pathways
- Multiomics Analysis
- Genome Annotation
- Epigenetic Modification

Protein Design



- Structure Prediction
- De Novo Drug Design
- Modeling Allosteric Effects
- Polypharmacology

Chemistry



- Design specific inhibitors
- Find potential energy states
- Simulate molecules
- Drug Discovery

Pharmaceutical R&D Process

Discovery

Target ID & Verification	Hit Generation	Lead Gen & Optimization	Pre-Clinical
1-2 yrs	1-2 yrs	1-2 yrs	1 yr

IND submitted

Development

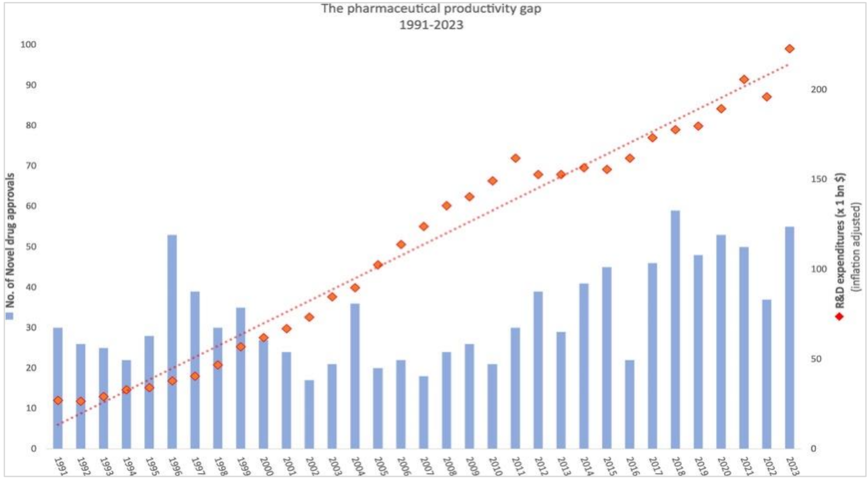
Phase 1 Safety	Phase 2 Safety & Efficacy	Phase 3 Safety & Efficacy	FDA Review & Approval
1-2 yrs	1-2 yrs	2-3 yrs	1-2 yrs

NDA submitted

Drug Discovery & Development Challenges

- **$ 3B** — Discovery Cost new drug 2024
- **10-15 Years** — Time to Market
- **90%** — Clinical drug development failure rate

Source :https://doi.org/10.1016/j.apsb.2022.02.002



Source: https://doi.org/10.1016/j.drudis.2024.104160

💻 CC: Classical-Classical

Classical Data → Classical Processing

Machine Learning based on methods borrowed from Quantum Information research, or "Quantum-Inspired" algorithms.

Examples: Tensor networks, quantum-inspired optimization

🔬 CQ: Classical-Quantum

Classical Data → Quantum Processing

Synonym for QML. Data come from classical systems like text, images, time series, macro-economic variables.

Key Challenge: Requires Quantum-Classical interface

🤖 QC: Quantum-Classical

Quantum Data → Classical Processing

How can Machine Learning help with Quantum Computing?

Examples: Quantum error correction, quantum state tomography

⚛️ QQ: Quantum-Quantum

Quantum Data → Quantum Processing

Closely related to CQ. Data can be measured from quantum systems or datasets can be Quantum States.

Examples: Quantum state classification, quantum sensing

Realistic Framing

What is "quantum for healthcare and life sciences"

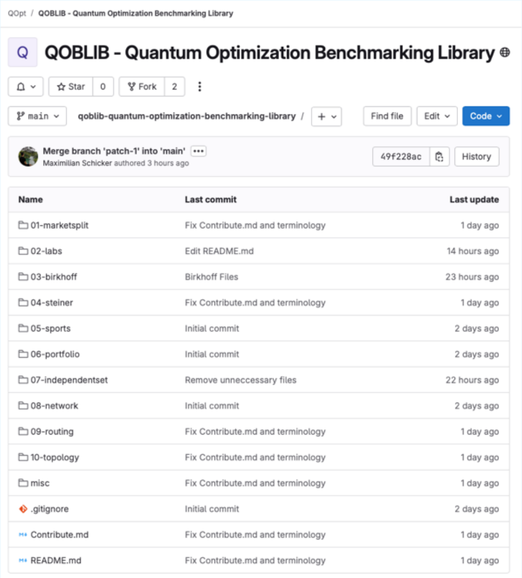
Today: noisy hardware → focus on careful benchmarking + hybrid workflows

Near-term: specialized wins where structure/scale stresses classical methods

Long-term: utility as hardware improves + better algorithms/compilation

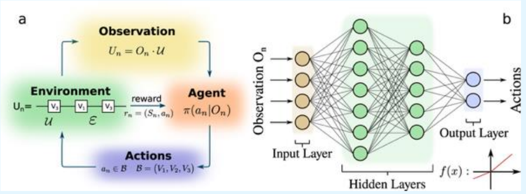
Opportunities to bring AI + Quantum together

- Benchmarking traditional, AI, and quantum approaches



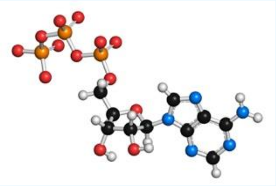
Critical for assessing computational problems

- AI functions to enable quantum workflows



- Compilation and circuit optimization
- Hyper-parameter turning
- Quantum algorithm discovery

- Quantum inputs into AI workflows

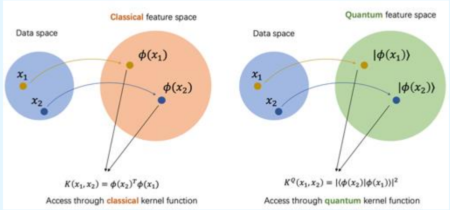


$H(x)$ → Quantum experiments → Classical ML

- Hybrid generative models for material discovery
- Quantum experiments + classical ML for property prediction

Leveraging quantum and AI to address larger scale problems

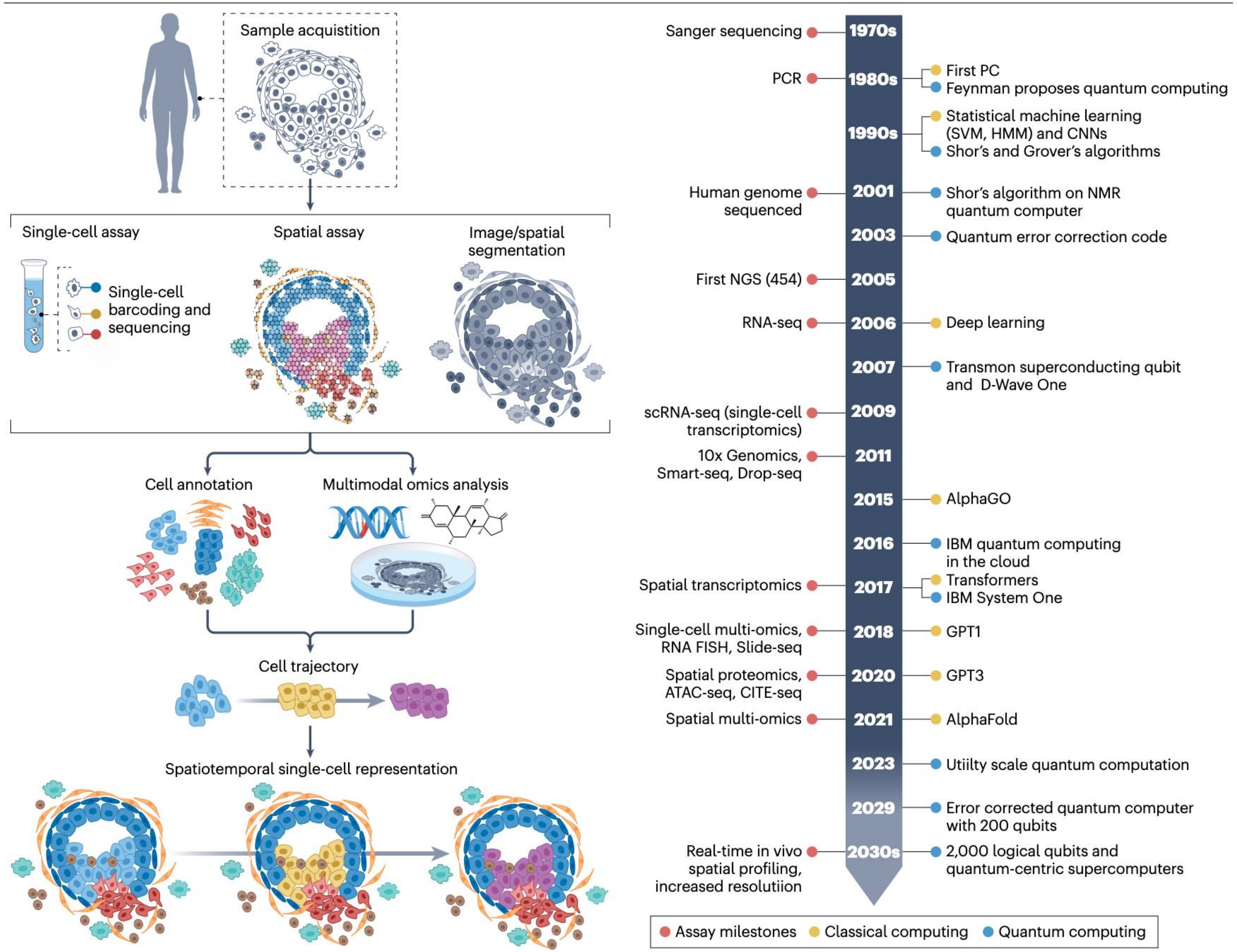
- Foundational algorithm development combining quantum and AI



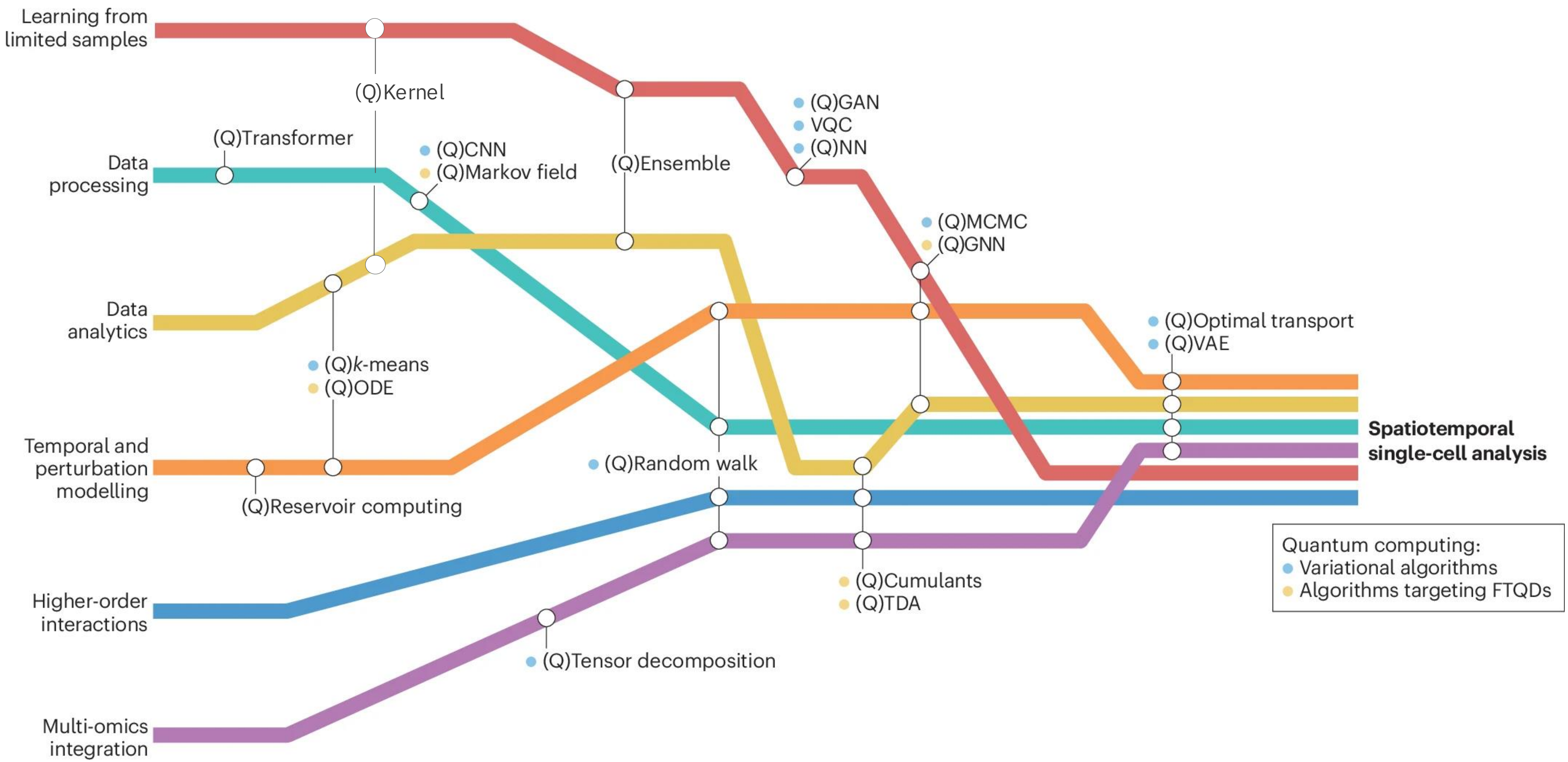
- Quantum enhanced learning (Quantum Kernels)
- Ensemble learning
- Novel representations

Transformational research for solving new problems

A timeline of discoveries in Life Sciences, AI, and Quantum



Classical and Quantum algorithms for single-cell analysis



Classical and Quantum Random Walks

Continuous-time Random Walk

Algorithm Variations
Classical & Quantum

Classical

$$\mathbf{P}(t) = e^{-t\mathbf{M}}$$

$$p_{uv}(t) = \mathbf{P}(t)[u, v]$$

Quantum

$$\mathbf{Q}(t) = e^{-it\mathbf{H}}$$

$$p_{uv}(t) = |\mathbf{Q}(t)[u, v]|^2$$

Discrete-time Random Walk

Algorithm Variations
Classical & Quantum

Classical

$$p_{j \to k} = P(X_{n+1} = k \,|X_n = j)$$

$$X_n = \sum_{k=0}^{n-1} \eta_k$$

Steps taking $+1$ or -1 with $p = \frac{1}{2}$

Quantum

$$p_{j \to k}(t) = \sum_{k=1}^{d_j} |\psi_{j,k}(t)|^2$$

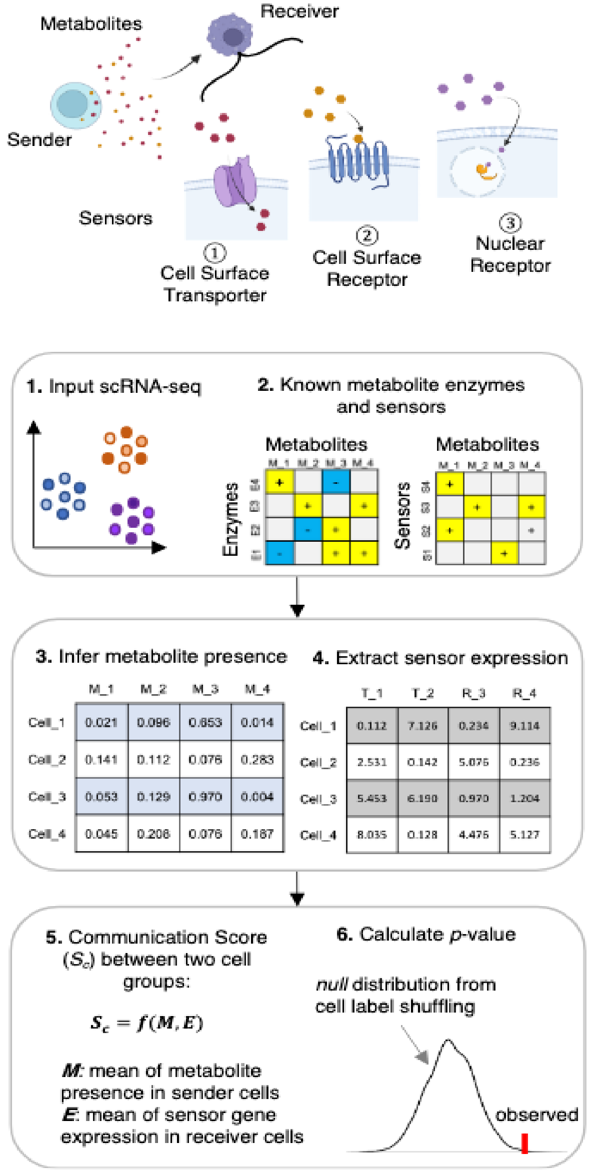
$$|\psi(t)\rangle = U^t |\psi(0)\rangle$$

$$U = SC$$

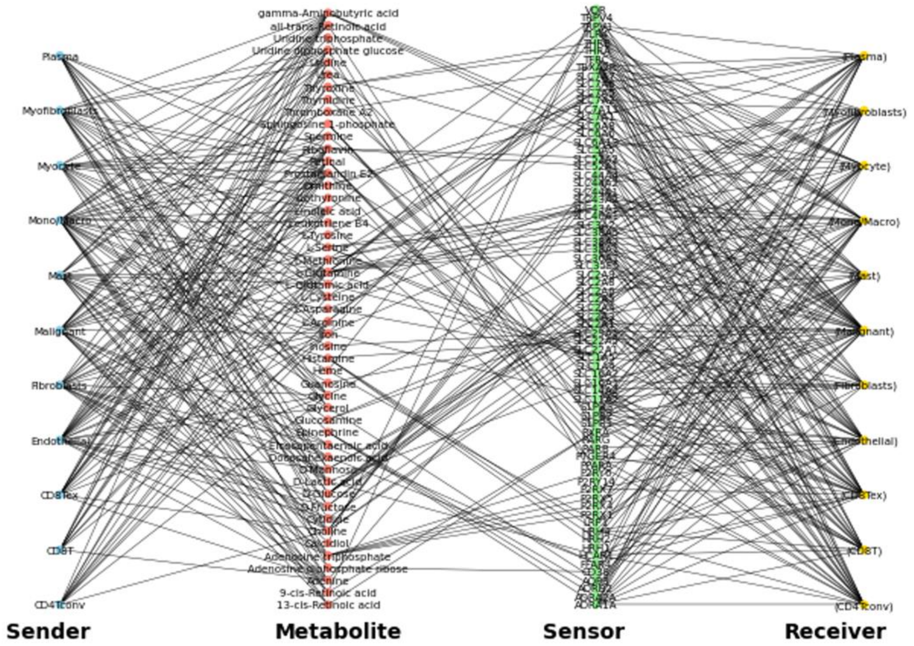
Shift operator

Coin operator

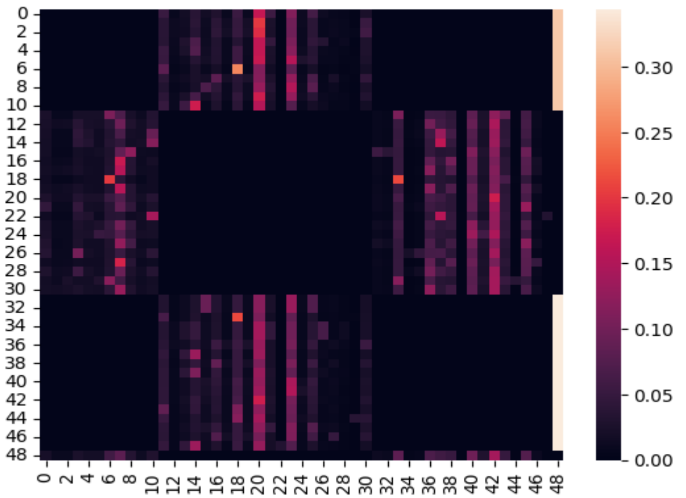
Quantum Random Wak in metabolic cell-cell interaction networks



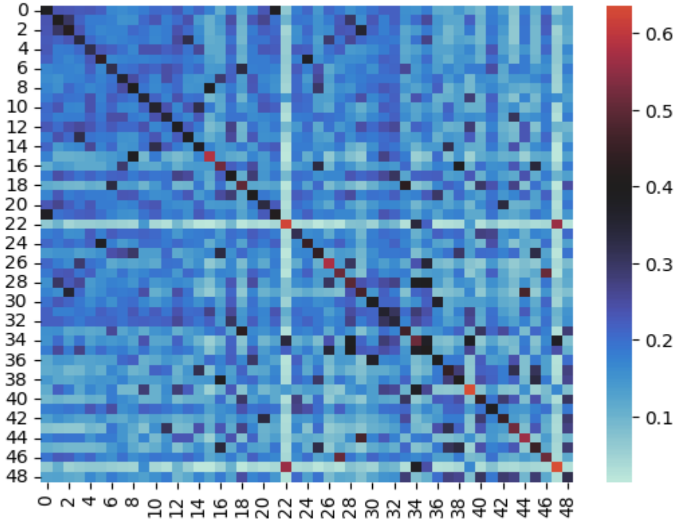
- Cell-cell interactions involving metabolites and sensor genes creates a multi-partite network from single-cell RNA-seq data of mouse brown adipose tissue (BAT)
- After five steps of evaluation the Euclidean distances between pairs of probability distributions recover five main communities in discrete-time random walk (DTRW), whereas in discrete-time quantum random walk (DT**Q**RW) there are more transitions between vertices in the CCI network.



Classical Random Walk

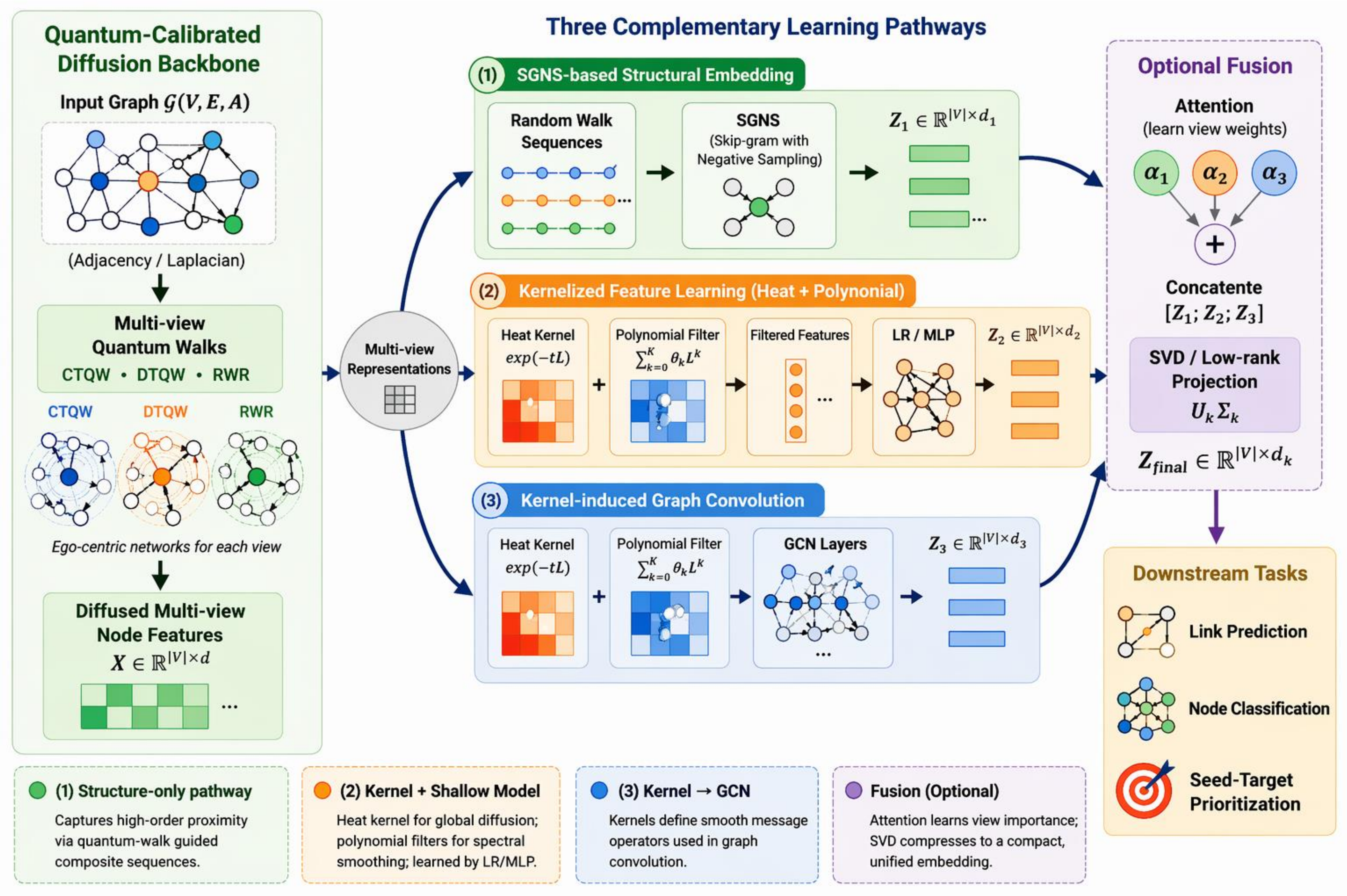


Quantum Random Walk

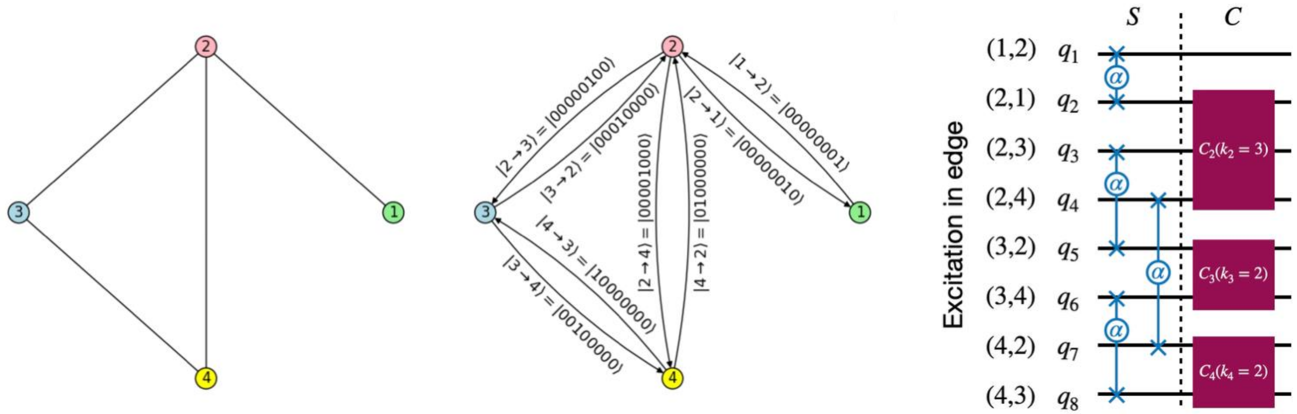


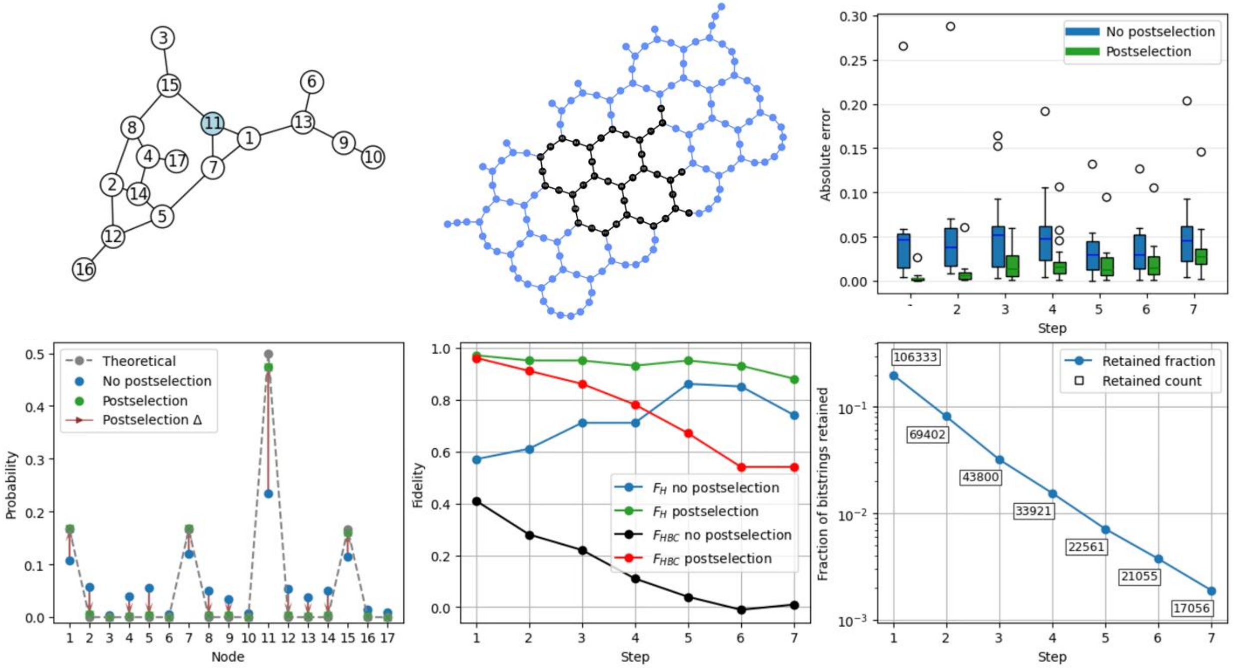
Dubovitskii et al. (2025) https://arxiv.org/abs/2506.06514

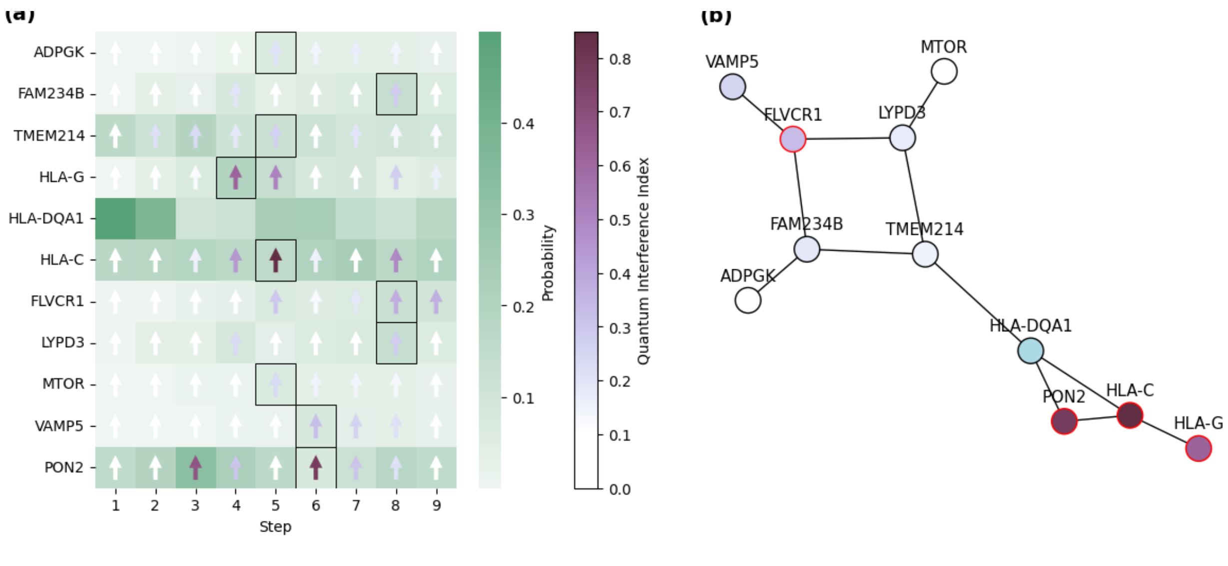
Quantum Graph Representation Learning



An implementation of Discrete-time Quantum Walk in Quantum Hardware



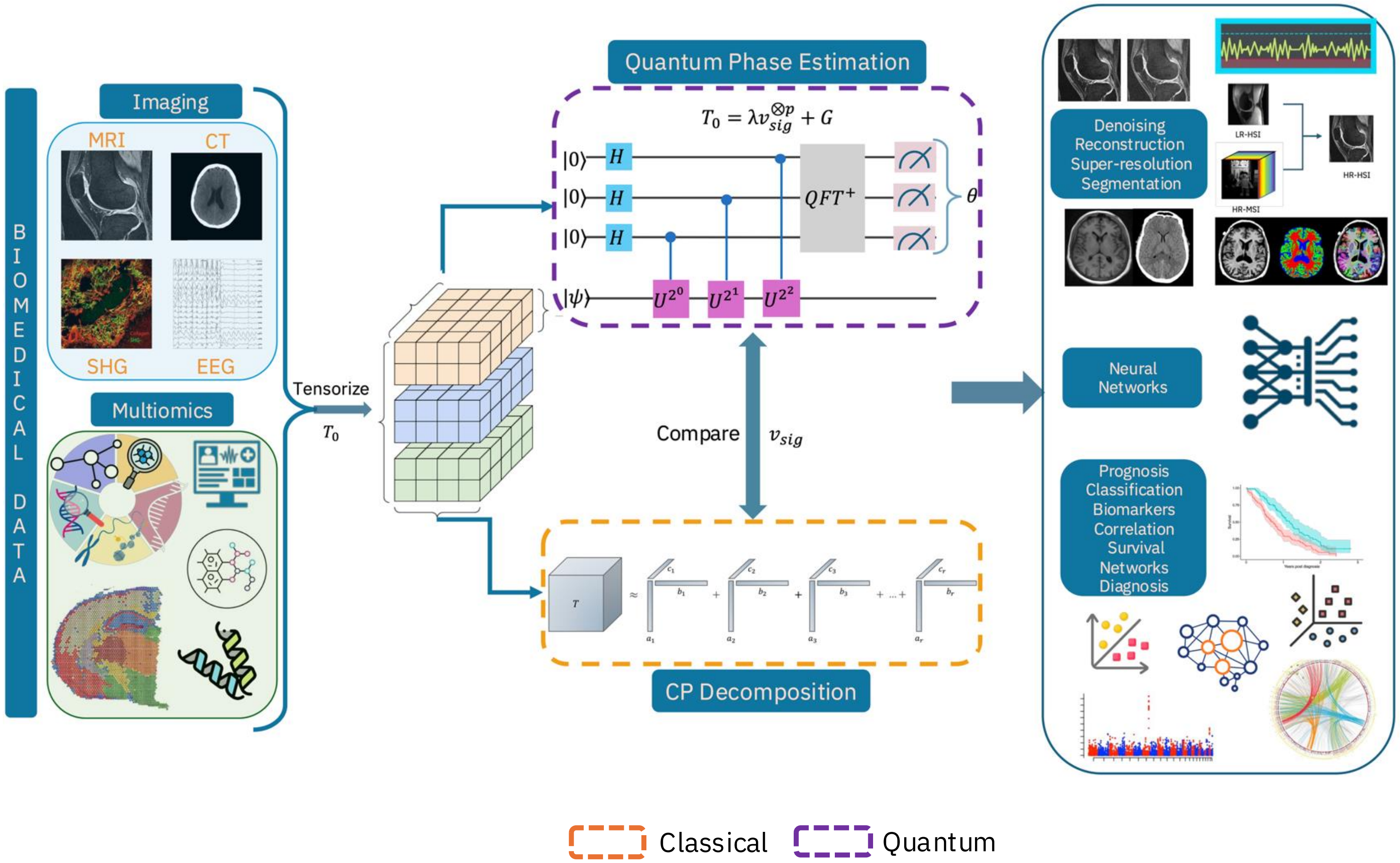


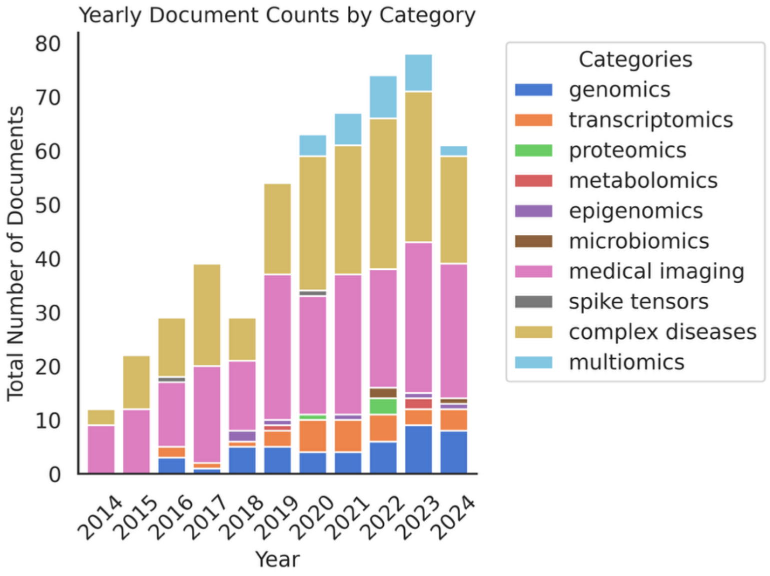


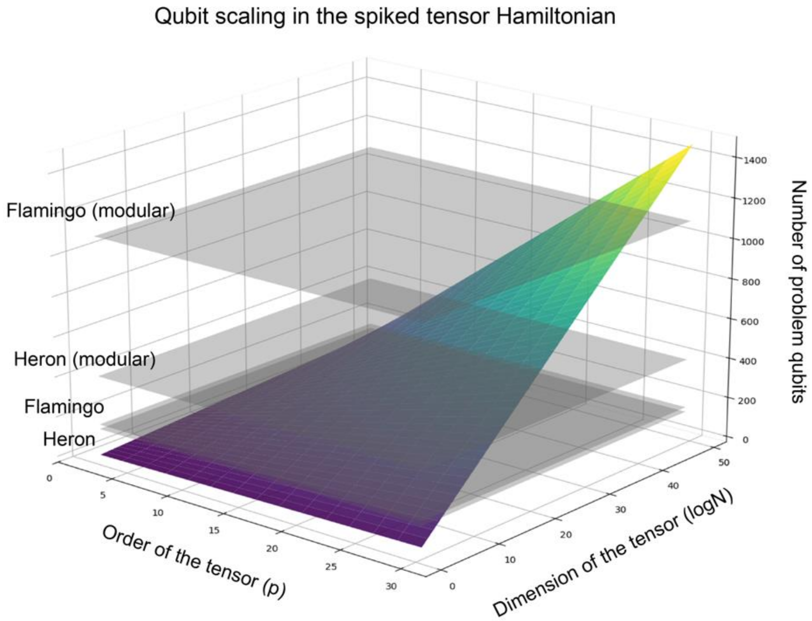
Dubovitskii et al. (2026) https://arxiv.org/abs/2602.24053

Quantum Tensor Decomposition for Biomedical Data

- Tensor decomposition is widely used in Biomedical data. It is NP-Hard and becomes intractable on a random tensor of size (N=100) and order > 4.
- Quantum tensor decomposition (QTD) has been shown to have a quartic speedup with provable guarantees. We are applying QTD on biomedical imaging data such as MRI, SHG, Spatial Transcriptomics, as well as in multi-omics data to accurately predict complex diseases.



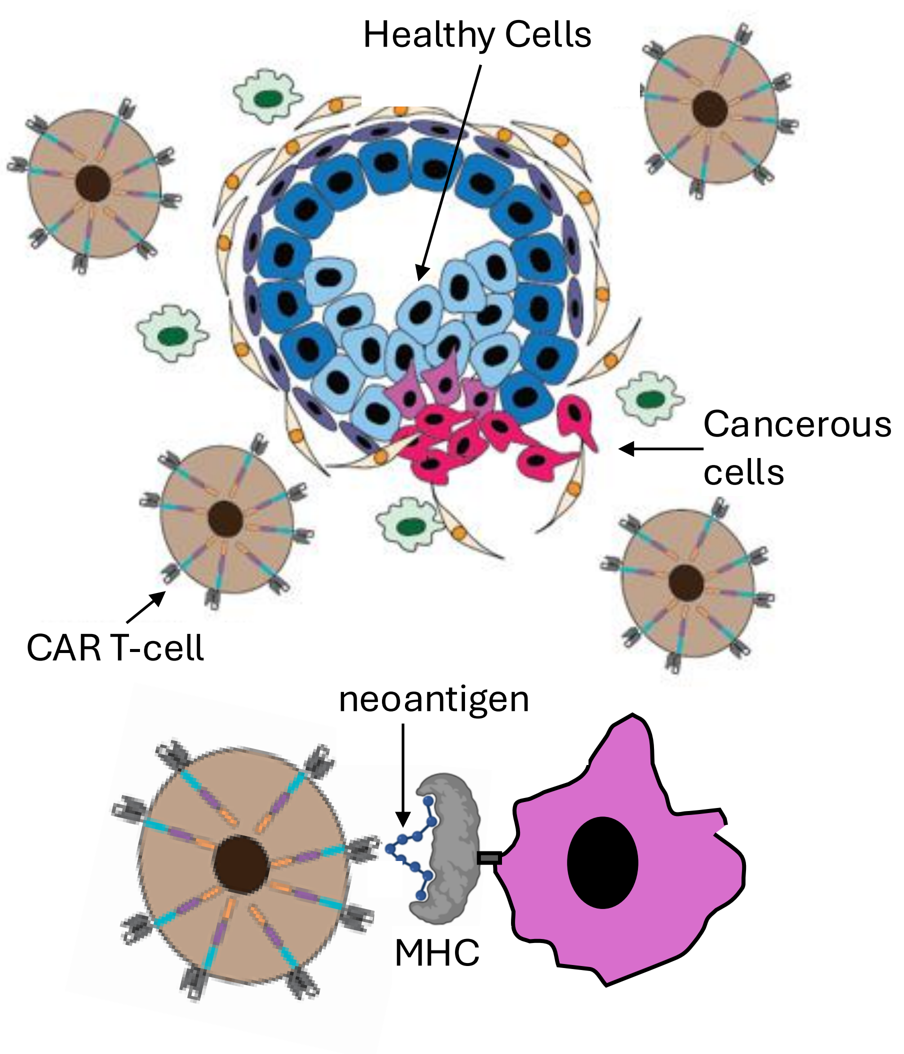




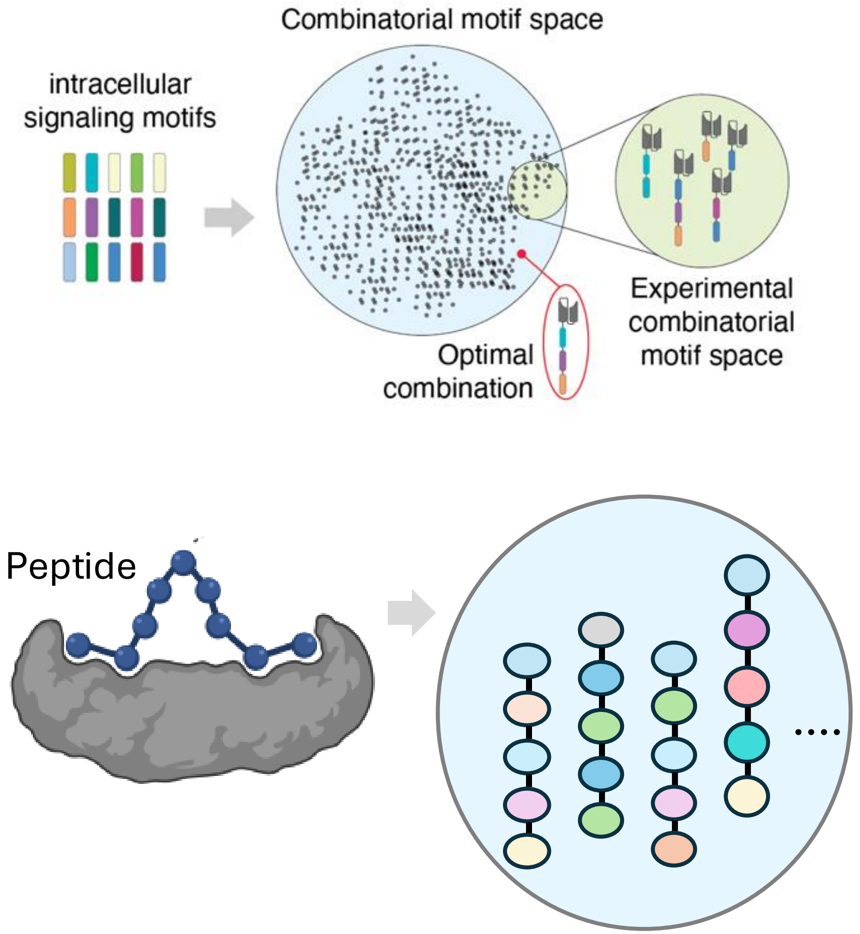
Burch et al. (2025) https://arxiv.org/abs/2502.13140

Quantum for ML – Applications in Immunotherapy

(A) Cell – protein interactions



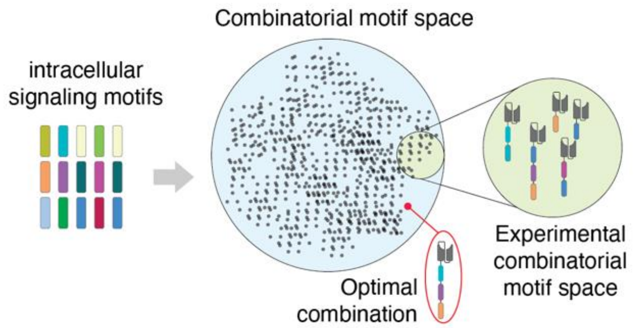
(B) Data space grows combinatorially



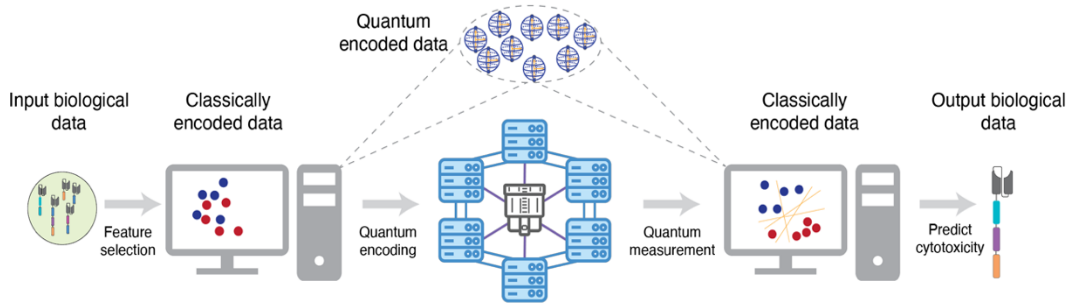
Data is experimentally generated; it is limited

Quantum for ML – Applications in Immunotherapy

Use-case 1: Identification of cytotoxic motifs

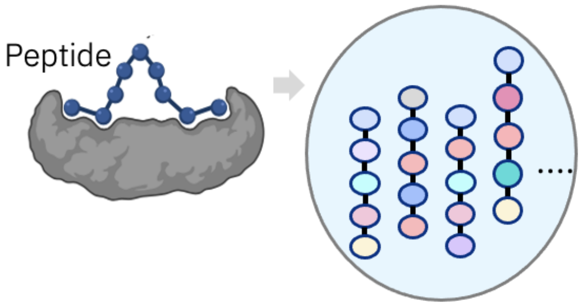


QML method: Projected Quantum Kernels

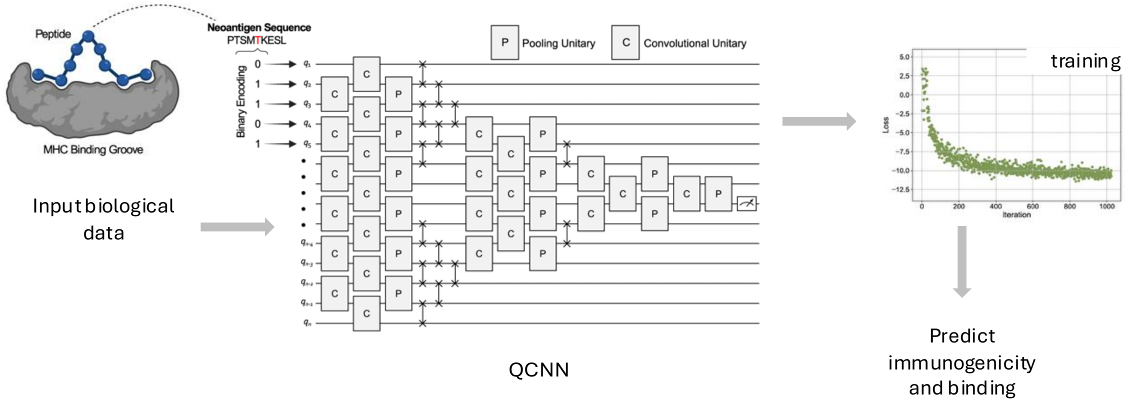


arXiv:2507.22710

Use-case 2: Predicting immunogenicity and binding



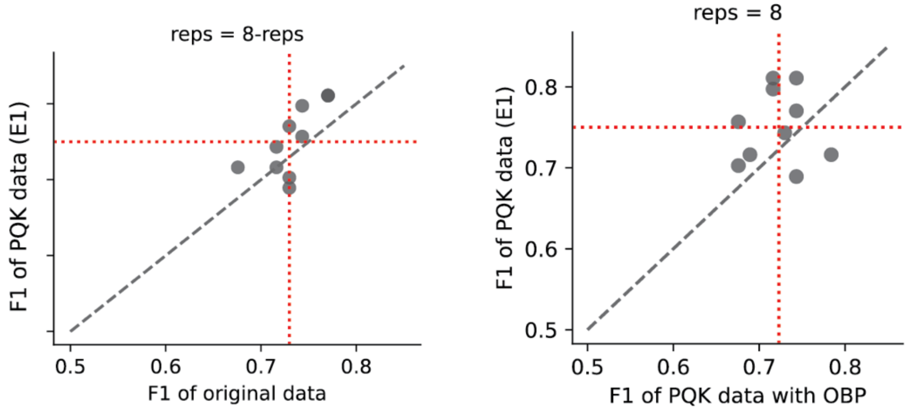
QML method: Quantum Convolutional Neural Networks



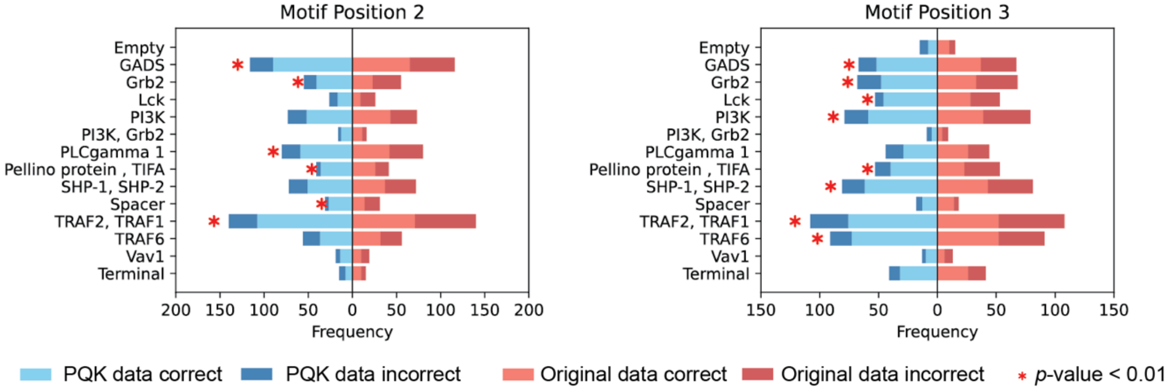
biorxiv:2025.07.29.667313v1

Quantum for ML – Applications in Immunotherapy

Use-case 1: Identification of cytotoxic motifs



Better prediction accuracy of the quantum model



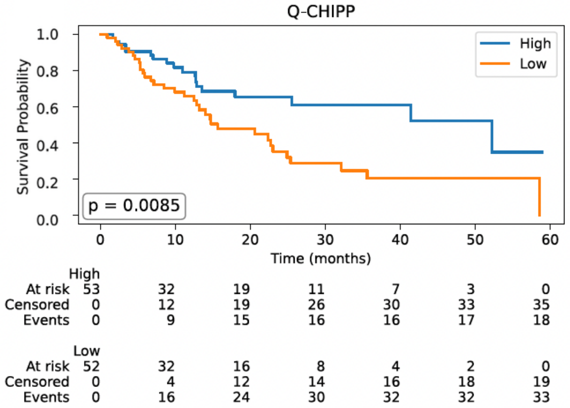
Quantum model provides unique biological insight

Utro et al. (2025) https://www.arxiv.org/abs/2507.22710

Use-case 2: Predicting immunogenicity and binding

Positions	QCNN	CNN (ltd.)	CNN (large)	RF
BA	**0.73**	**0.73**	**0.73**	0.68
1,4,5,9	**0.71**	0.33	0.67	0.64
1,4,5,9,BA	0.71	0.50	**0.72**	**0.72**
4,6,7,8	0.49	0.39	0.33	**0.52**
4,6,7,8,BA	0.54	0.35	0.68	**0.72**
4,6,8,9	0.70	0.35	**0.71**	0.68
4,6,8,9,BA	0.74	0.55	0.71	**0.77**
Full peptide	**0.70** *	0.60	0.65	0.66

QCNN model is better or comparable to classical ML models



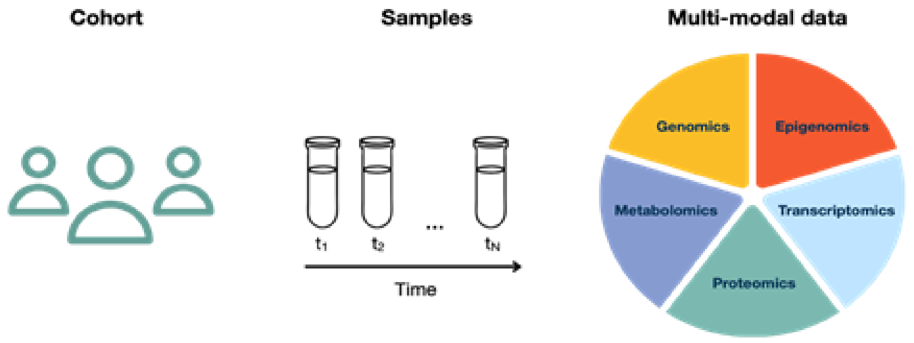
Survival predicted by the quantum model beats classical predictions

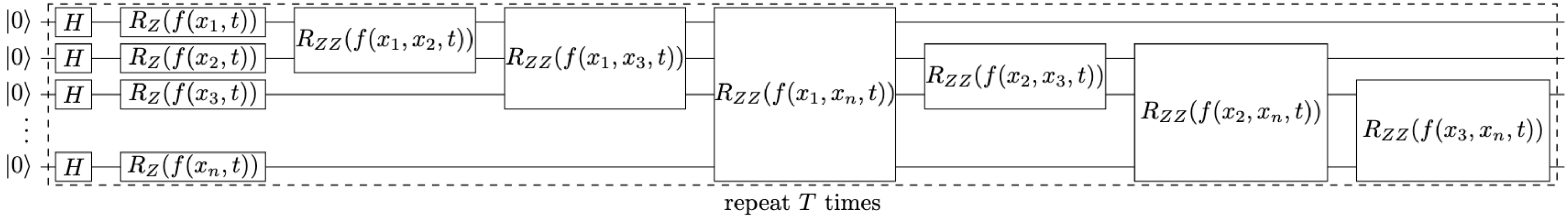
Peters et al. (2025) https://doi.org/10.1101/2025.07.29.667313

Quantum for ML – Longitudinal Biomedical Studies

The ability to capture changes in molecular profiles over time enabled observations of evolution of treatment response and/or progression in diseases.

We aim to develop a quantum computational methodology for longitudinal omics data analysis and investigate possible advances.





Demidik et al. (2025) https://arxiv.org/abs/2504.18392

Quantum Computing in Virtual Screening of Drug Candidates

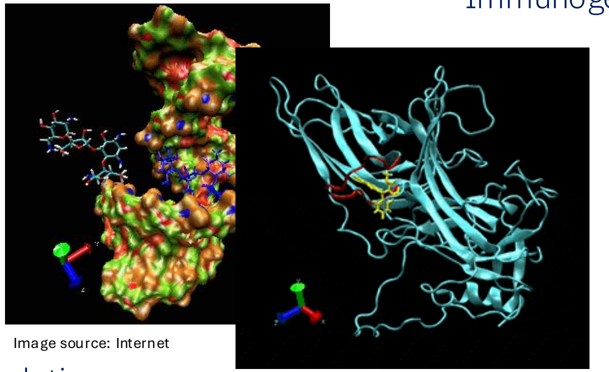
Target ID & Verification → Hit Generation → Lead Gen & Optimization → Pre-Clinical → Phase 1 Safety → Phase 2 Safety & Efficacy → Phase 3 Safety & Efficacy → FDA Review & Approval

Clinical Development

Stability

Immunogenicity

Drug Delivery



Binding Affinity

Image source: Internet

Formulation Development

Synthesizability

- Small molecules
- Oligonucleotides
- Peptides
- Enzymes
- Antibodies
- Cell Therapy
- Stem Cell

Biologics

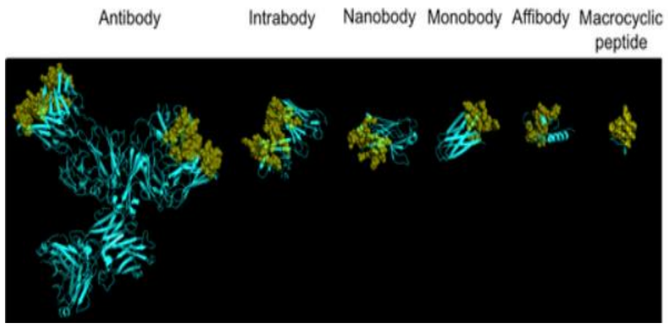


Image source: Internet

Chemical Space: 20^K

K = number of residues

Classical computer

With a Force Field:

Less Accuracy

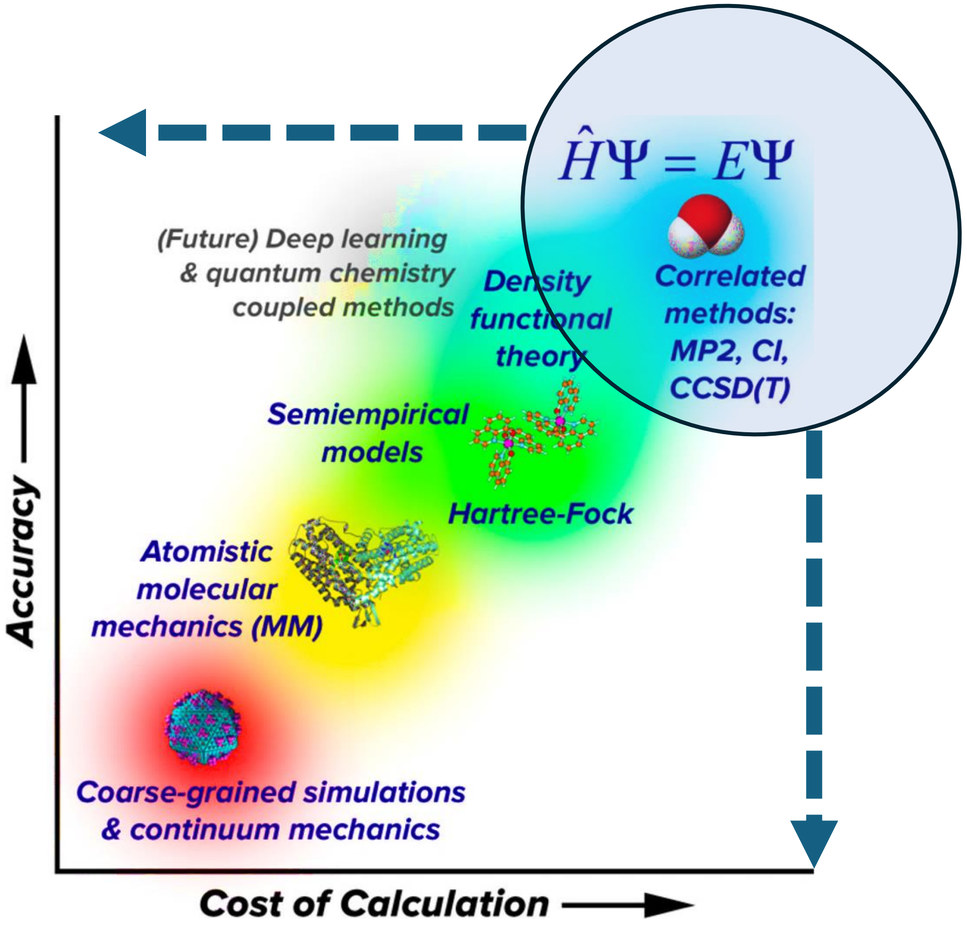
Quantum computer

With Quantum Simulations:

More Accuracy

Multi constraint – multi-objective optimisation problem

Quantum Computing in Virtual Screening of Drug Candidates



Source: Chem. Rev. 2021, 121, 10, 5633-5670

FT

- Quantum Phase Estimation
- Quantum Amplitude Estimation

NISQ

- Variational Quantum Eigensolver
- Quantum Approximate Optimization Algorithm

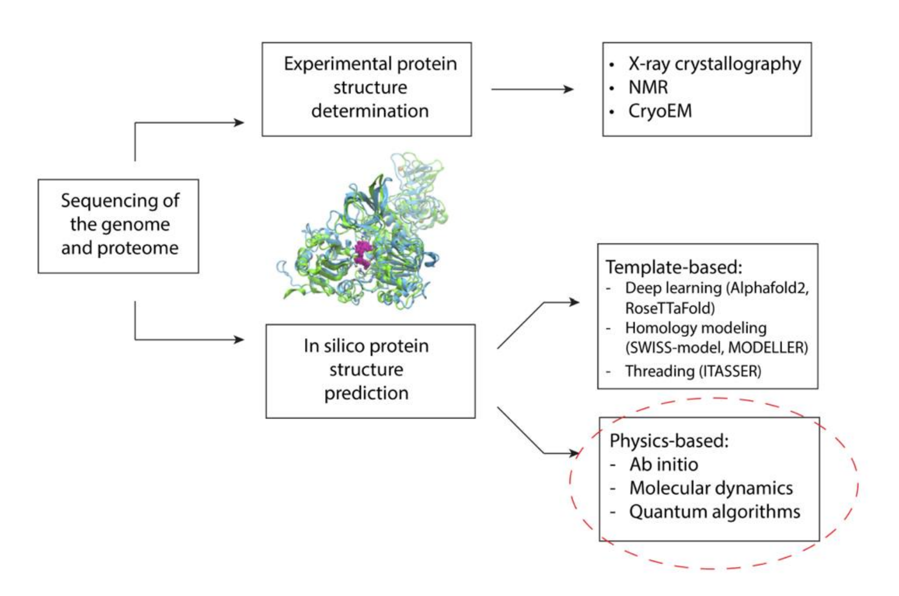
Quantum Computing Applications

- Accurate Simulation of Supramolecular Interactions
- Accurate Binding Energy Calculation
- Ligand Design & Lead Optimization

Case Study with Cleveland Clinic (Protein Folding)

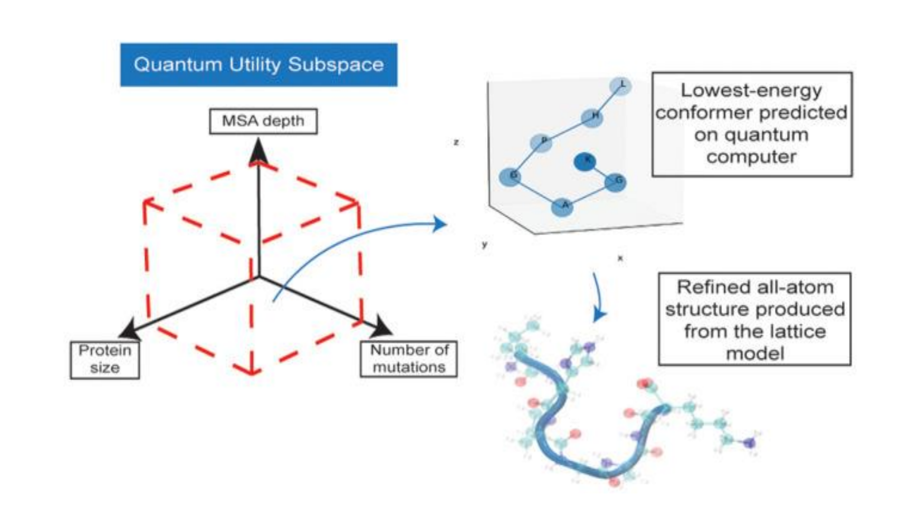
Problem

Predicting protein structures is critical for creating new biological products, but classical deep learning struggles with mutated sequences, IDRs, and low MSA depth.



Quantum Method

Hybrid quantum-classical algorithms, like VQE and QAOA, improve native protein structure identification, addressing classical limitations.



Doga et al. https://arxiv.org/abs/2312.00875
Robert et al., https://www.nature.com/articles/s41534-021-00368-4

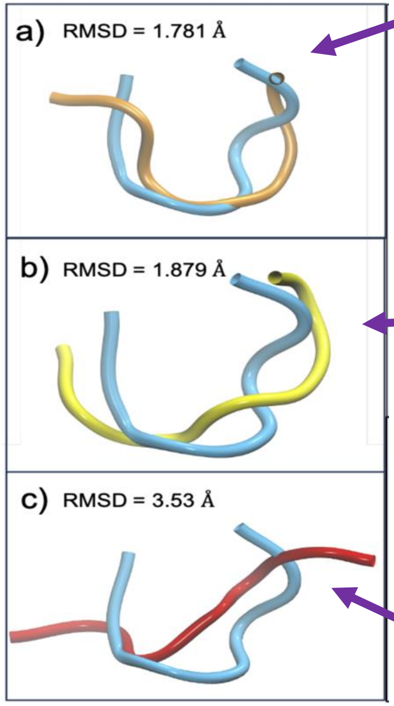
Case Study with Cleveland Clinic (Protein Folding)

Method:

VQE model is used to accurately predict the structure of a 7 amino acid catalytic loop of the Zika Virus NS3 Helicase.

Solution:

Quantum optimization can advance protein structure prediction, driving innovations in biological product design and therapeutic development.



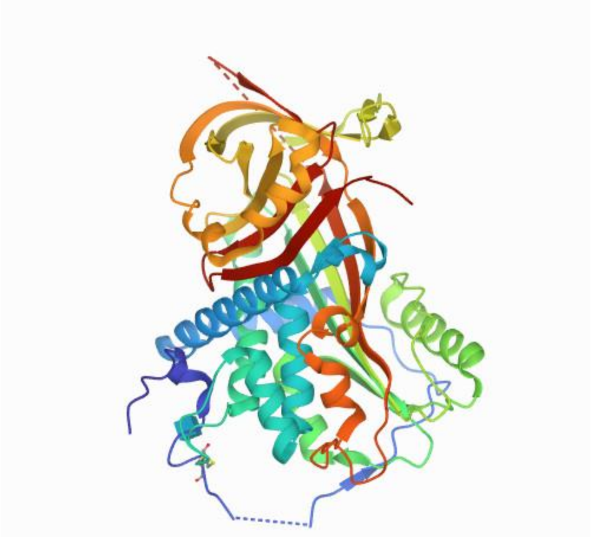
VQE

Brute force

AlphaFold2

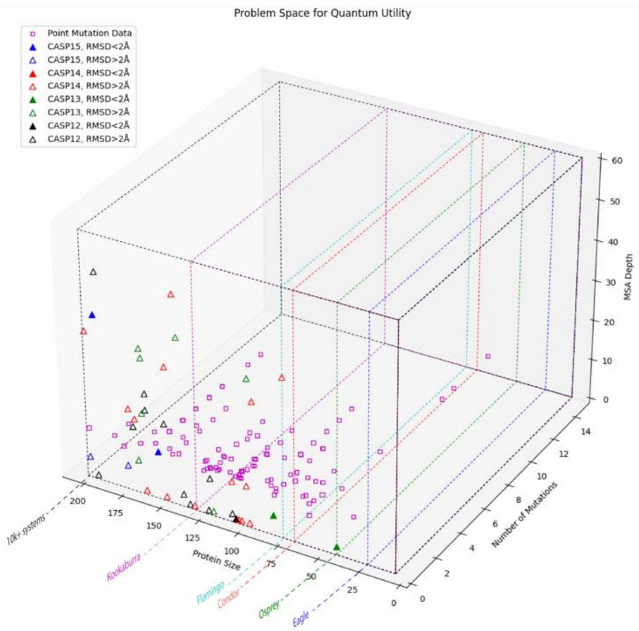
7 amino acid protein is mapped to 9 qubits on the IBM Cleveland quantum computer

Doga et al. https://pubs.acs.org/doi/10.1021/acs.jctc.4c00067



10 amino acid Angiotensin peptide on 22 qubits

Robert, A. et al. https://doi.org/10.1038/s41534-021-00368-4



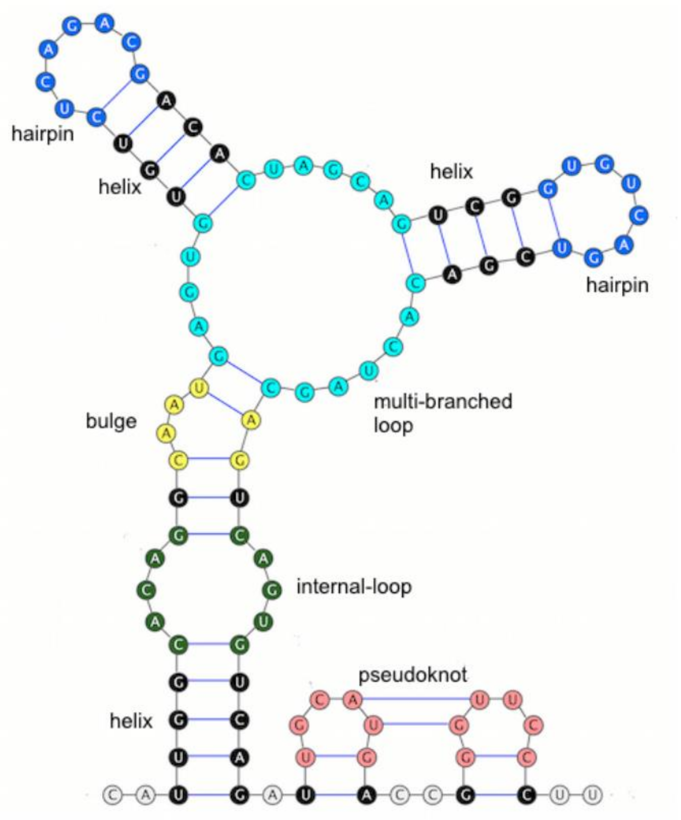
Case Study with Moderna (mRNA Structures Prediction)

Problem:

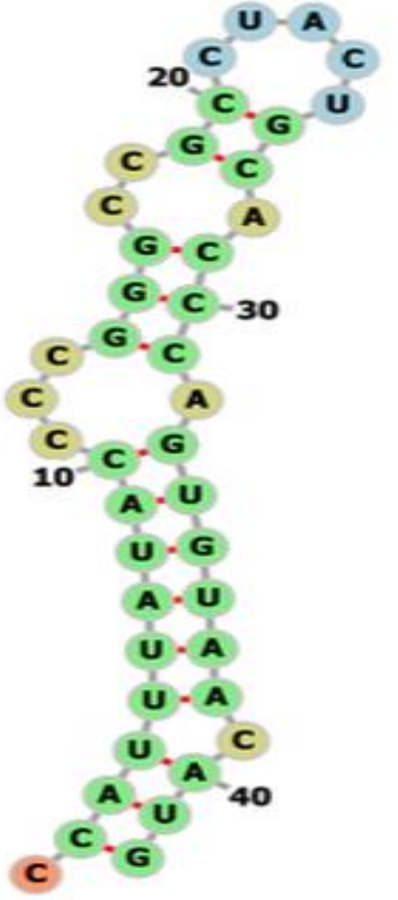
Predicting mRNA secondary structures is a formidable combinatorial optimization problem due to the vast number of possible configurations and their associated energy states.

Solution:

Results indicate that quantum computing offers valuable insights into RNA folding mechanisms and enables rapid identification of functional RNA structures. This work lays the groundwork for future research in quantum-assisted bioinformatics and highlights the importance of developing scalable quantum algorithms for real-world biological problems.



An RNA secondary structure illustrating five kinds of secondary structural elements: hairpin loops (blue), bulge (yellow), helix (black), internal loop (green) and multi-branched loop (cyan) and a pseudoknot (pink)

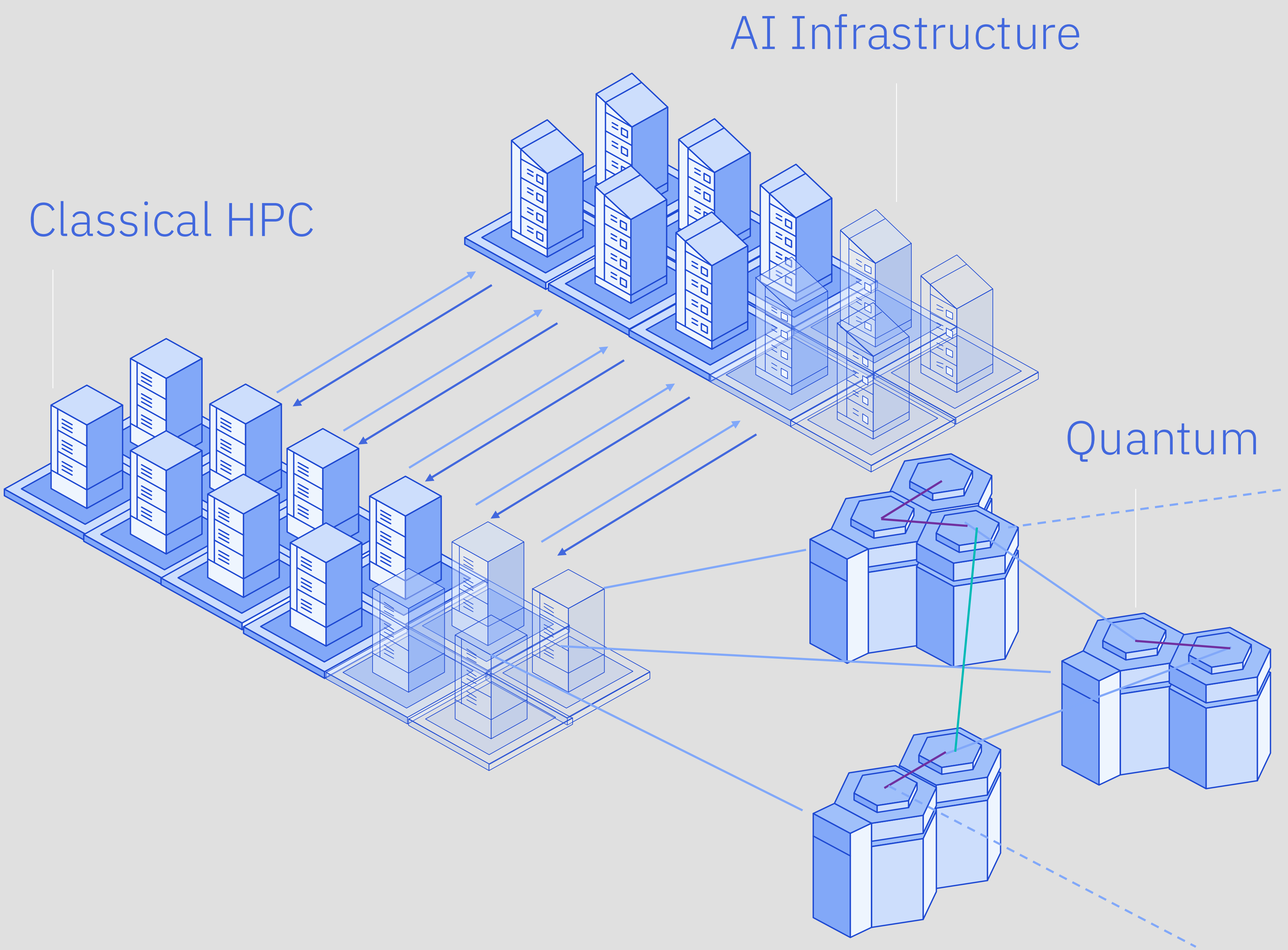


Optimal folded structure of the 42- nucleotide mRNA sequence on 80-qubit based on the corresponding lowest energy bitstring found by the hardware run.

Alevras et al., https://arxiv.org/pdf/2405.20328

Next Generation Computing

Bits + Neurons + Qubits

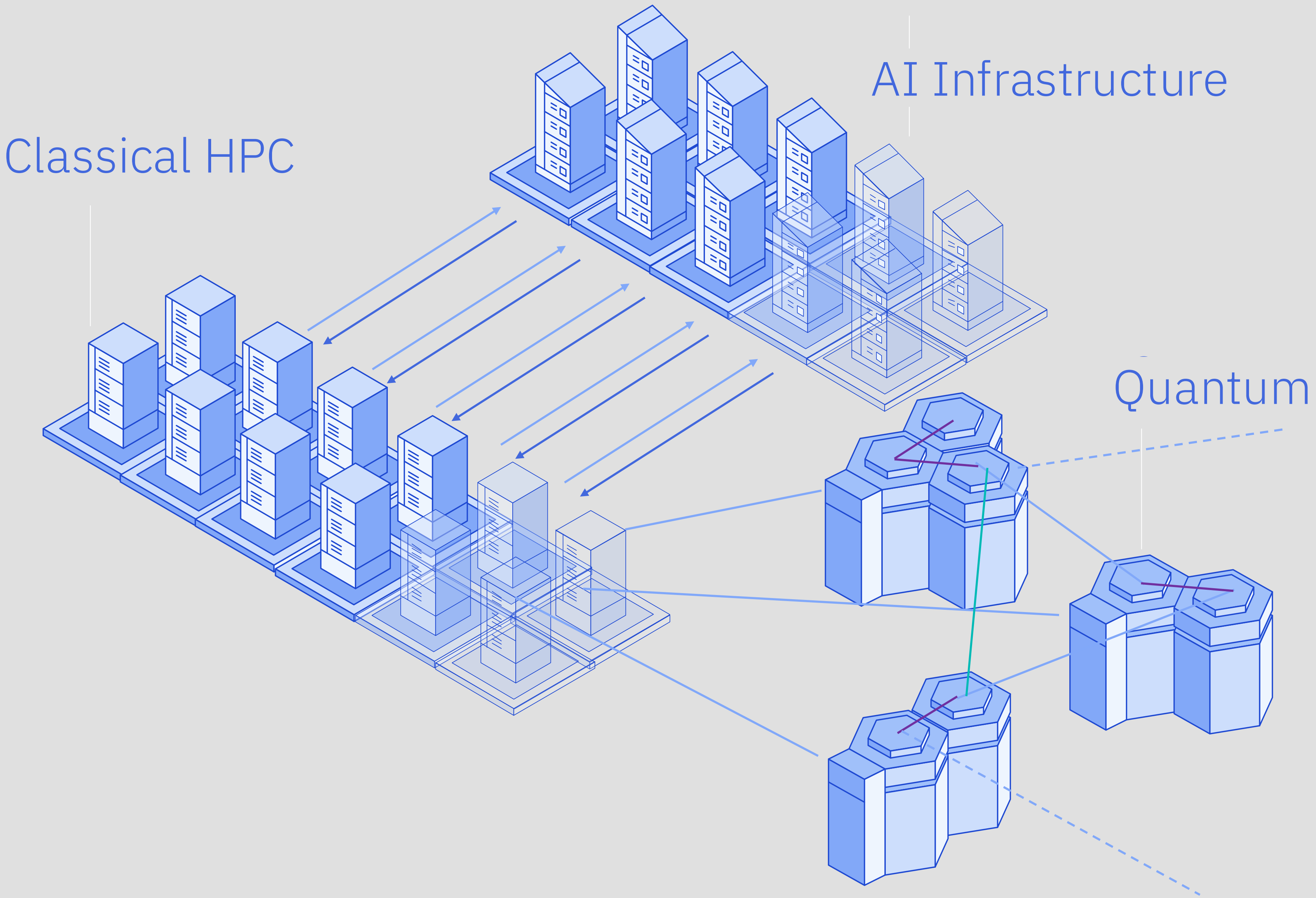


Bits + Neurons + Qubits

Future of Computing: Quantum Centric Supercomputing

IBM's Quantum-Centric Supercomputing (QCSC) — merges classical and quantum systems, paving the way for solving pharma-relevant problems that are intractable today — with chemistry quantum advantage expected by 2026.

Early quantum integration builds strategic advantage — enabling pharma companies to shorten the learning curve, develop in-house quantum expertise, and position themselves as leaders in next-gen R&D innovation.



Quantum-centric Supercomputing Integration at RIKEN (R-CCS)

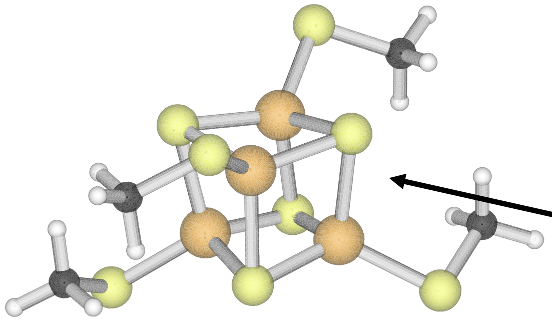
RIKEN Fugaku supercomputer

IBM Quantum System Two

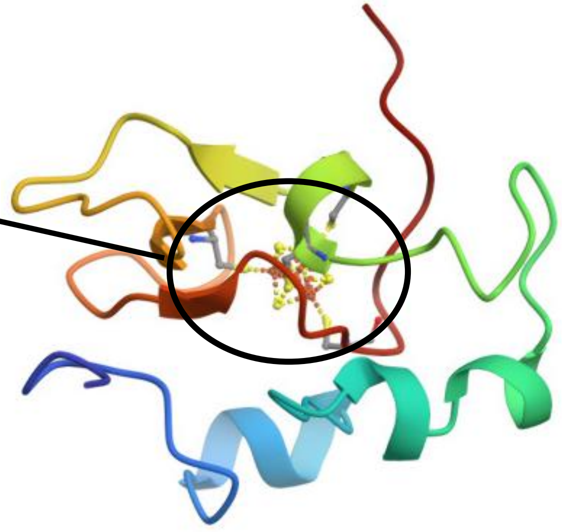
Planned deployment 2Q 2025
Infiniband 400 Gb/s
Co-located
⟷

Quantum Chemistry on Pre-Fault-Tolerant Devices:

Sample-based quantum diagonalization (SQD)



[4Fe-4S] on a 36-orbital active space:
72 qubits



Fault-tolerant	Phase estimation qubits: **4.53M** **13 days** *
Pre-fault tolerant	VQE estimation at 10μs/circuit ~**3M years**
Quantum-centric supercomputing	Subspace estimation at 10μs/circuit ~**2 hours**

*Estimation done using surface code

Density Matrix Embedding Theory (DMET) + SQD

Applications in Drug Design

Understanding Protein Function
Designing Specific Inhibitors
Predicting Cluster Reactivity

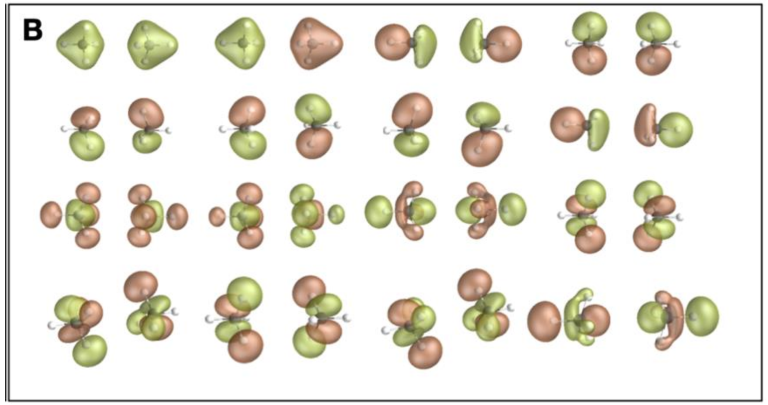
arXiv:2405.05068 (2024)

https://www.ibm.com/quantum/case-studies/modeling-realistic-chemistry#demo

Industry Applications of Sample-based Quantum Diagonalization (SQD)

Cleveland Clinic

Simulate the potential energy surfaces (PES) of the water and methane dimers (hydrophilic and hydrophobic interactions)

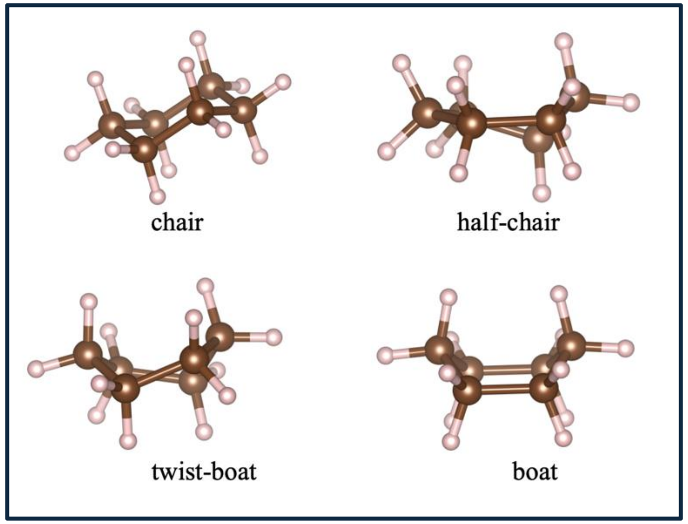


54 qubits, 1600 2Q gates

arXiv:2410.09209

Cleveland Clinic

Simulation of relative energies of cyclohexene conformations



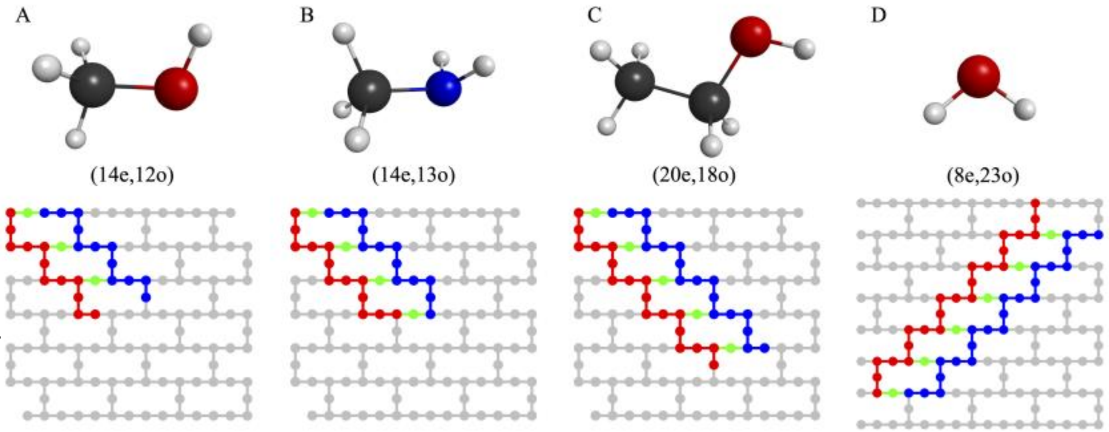
41 qubits, 1500 2Q gates

arXiv:2411.09861

Cleveland Clinic

SQD based simulation of
A. Methanol
B. Methylamine
C. Ethanol
D. Water

Qubit layouts of Local Unitary Cluster Jastrow (LUCJ) circuits. Qubits used to encode occupation numbers of spin-up/down electrons are marked in red/blue, while ancilla qubits denoted in green.

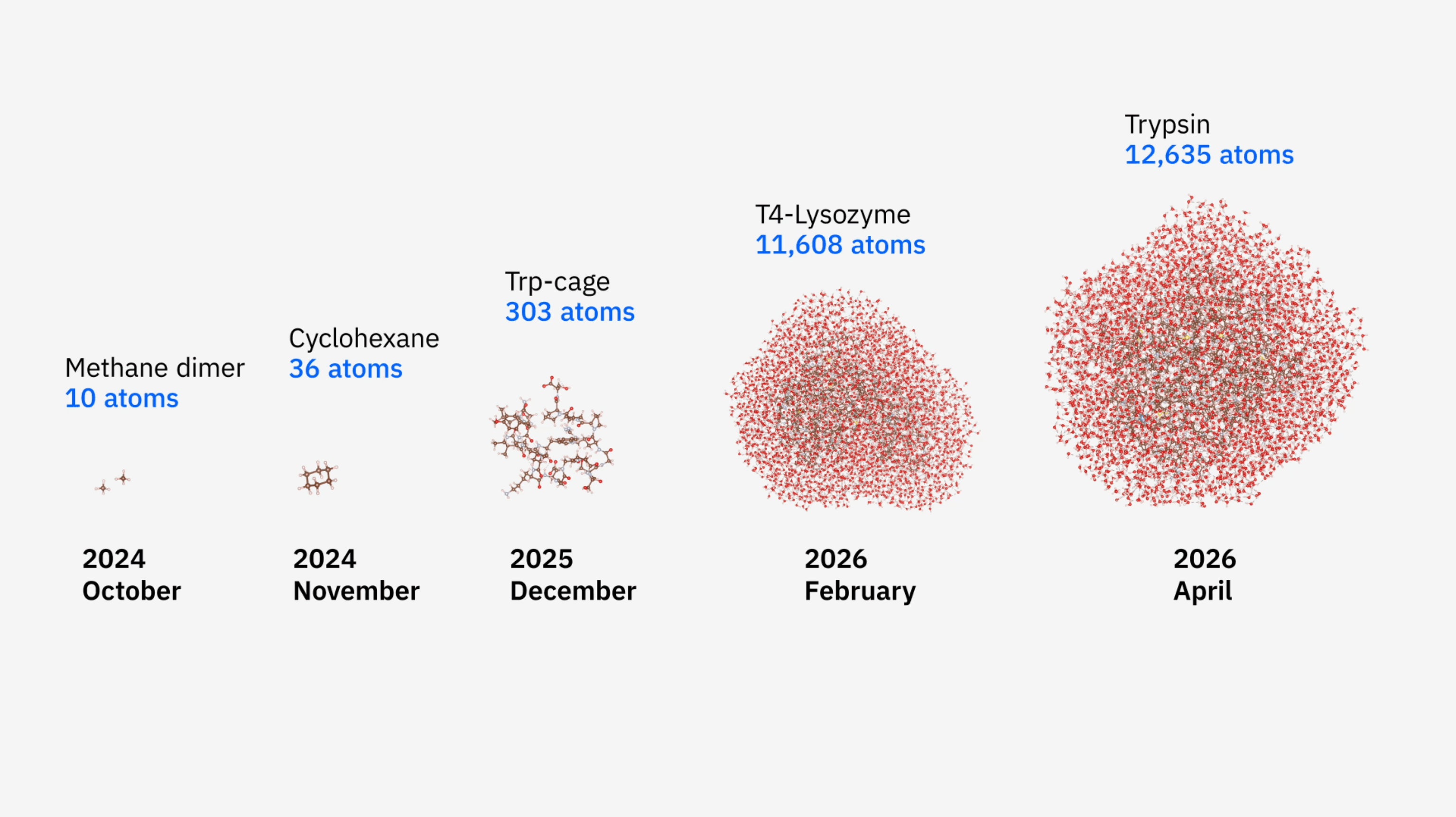


27 qubits | 30 qubits | 41 qubits | 52 qubits

arXiv:2502.10189

Researchers use quantum-centric supercomputing to simulate 12,635-atom protein complex

A team from Cleveland Clinic, RIKEN, and IBM used two IBM quantum computers and two supercomputers to model biologically relevant molecules at scale.



arXiv:2605.1138

Thank you.

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Thank you!