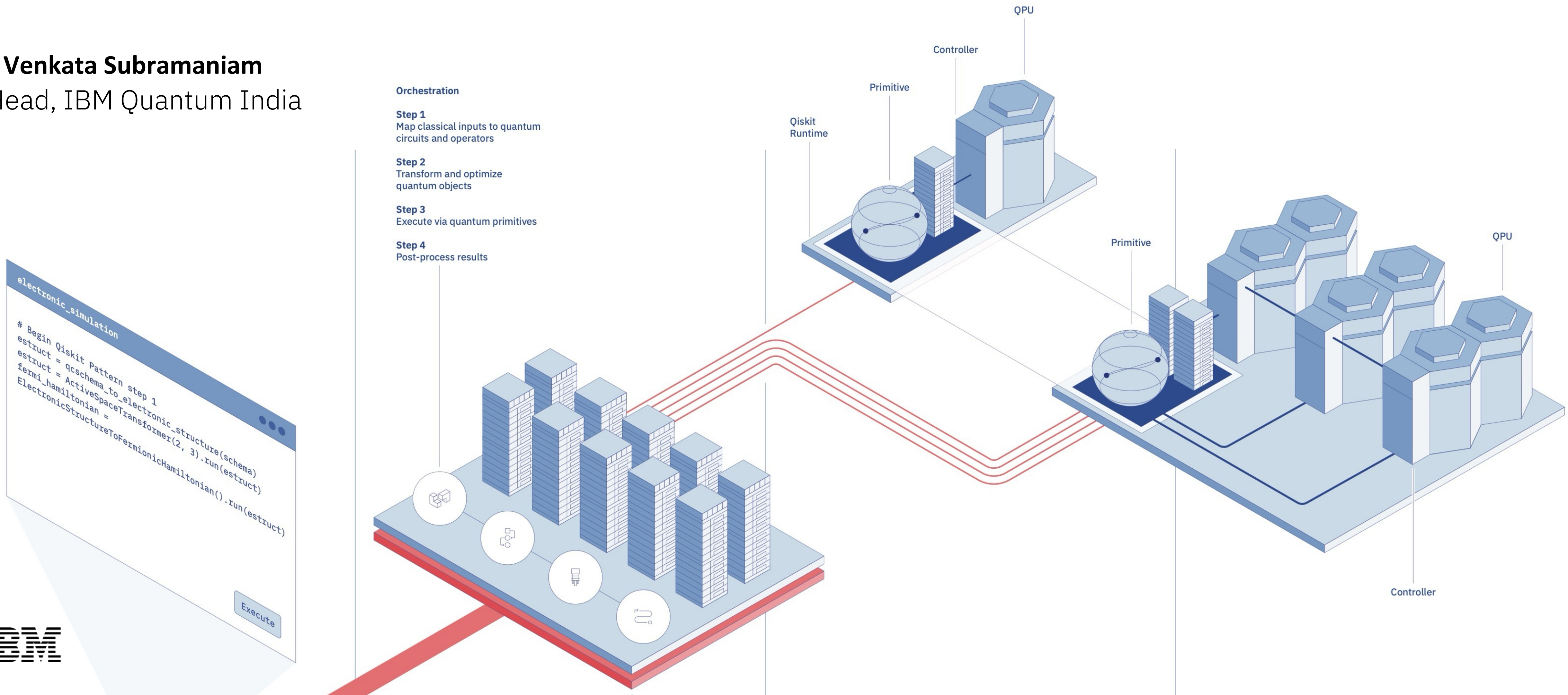
Quantum Decade: India’s Leap Forward

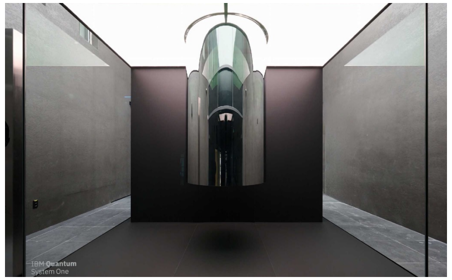
L Venkata Subramaniam
Head, IBM Quantum India



New and planned on-prem installations

5

Quantum Computational Center
Yonsei University
Seoul, South Korea
November 2024



JHPC-quantum
RIKEN
Kobe, Japan
June 2025

IBM-Euskadi Quantum Computational Center
San Sebastián, Spain
Projected September 2025

National Quantum Algorithm Center
Chicago, Illinois
Projected December 2025

Quantum Valley Tech Park
Andhra Pradesh, India
Projected 1Q 2026

Facilitating algorithm discovery through public investments

National Quantum Algorithm Center

Chicago, Illinois

In December 2024, IBM and Illinois Governor JB Pritzker announced a collaboration to establish the National Quantum Algorithm Center in Chicago, anchored by an IBM Quantum System Two, to drive advances in utility-scale algorithm research.

Quantum Valley Tech Park

Andhra Pradesh, India

In May 2025, IBM and Tata Consultancy Services announced their partnership to deploy an IBM Quantum System Two in the State of Andhra Pradesh's Quantum Valley Tech Park and facilitate algorithm discovery by providing cloud-based access to scientists in the region.

IBM Quantum Platform: Software

Accelerate application research with a high-performance software stack powered by Qiskit

Qiskit SDK

Preferred by 74% of the developer community

4000+ dependent projects

63% faster mean transpilation time than nearest competitor TKET

Qiskit Runtime

Accurately and efficiently execute estimation and sampling tasks in a near-time environment

Quality: Up to 5K gates
Speed: 250k+ CLOPS

Qiskit Serverless

Run quantum-centric supercomputing workloads across QPUs, CPUs, and GPUs in the cloud

Simplifies heterogeneous application development for researchers

Don't just do, develop

Beginner

Qiskit Aer

Intermediate

Qiskit Ecosystem

Proficient

Qiskit Addon

Types of involvement

- Solve some existing issues, and submit a PR
- Enhance the software with new features
- Improve some algorithmic aspects of the software

  Add new research innovations as enhancements

- Work with IBM India researchers and interns in cutting-edge algorithms and development.
- For significant involvement, achieve a GRM certificate.
- Showcase your proficiency in quantum computing and software development skills during internship and job applications.

One of the world's most powerful supercomputer

IBM **Quantum**

Oak Ridge National Laboratory
US Department of Energy

Summit supercomputer specs

200 quadrillion calculations per second

9216 IBM Power 9 processors

27,648 NVIDIA GPUs

250 PB File System

IBM Red Hat Enterprise Linux (RHEL) v 7.4 Operating System

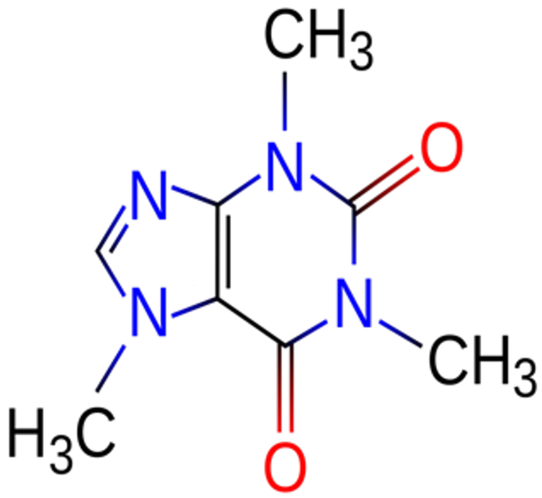
https://www.ibm.com/thought-leadership/summit-supercomputer/

Computing with caffeine

If our best classical computers are so powerful, shouldn't we be able to perfectly simulate molecules and chemical reactions?

This would allow us to accelerate discovery of new compounds and processes for healthcare, materials, alloys, and sustainable energy creation.

Let's consider caffeine ...



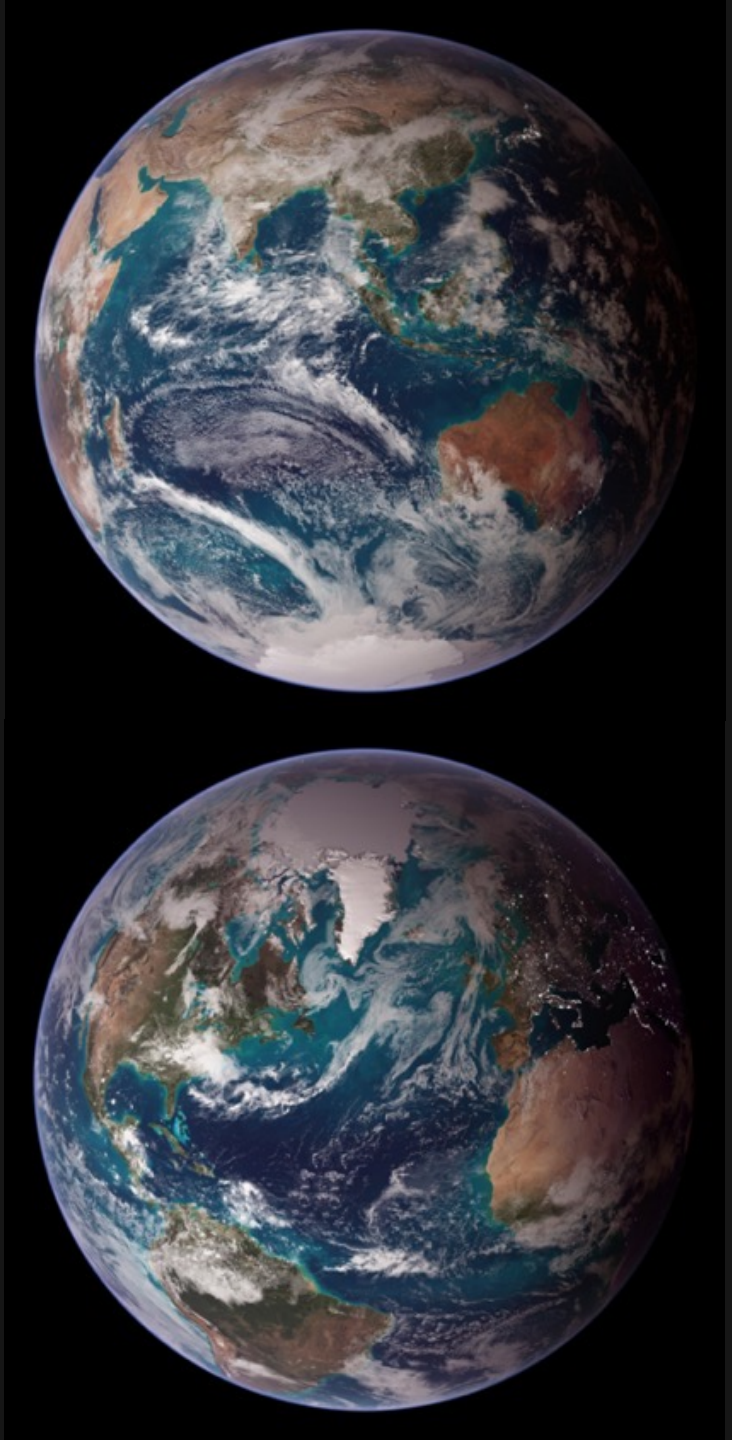
Computing with caffeine

We would need approximately 10^{48} bits to represent the energy configuration of a single caffeine molecule at a single instant in a classical computer.

This is 1 to 10% of the total number of atoms in the Earth.

10^{48} =

1,000,000,000,000,000,
000,000,000,000,000,000,
000,000,000,000,000



IBM **Quantum**

Computing with caffeine

Although it’s impossible to completely represent the molecular configuration of caffeine on today’s most powerful super computers, we could represent it using 160 logical qubits.

It takes a long time to develop new materials…

10-20+ years

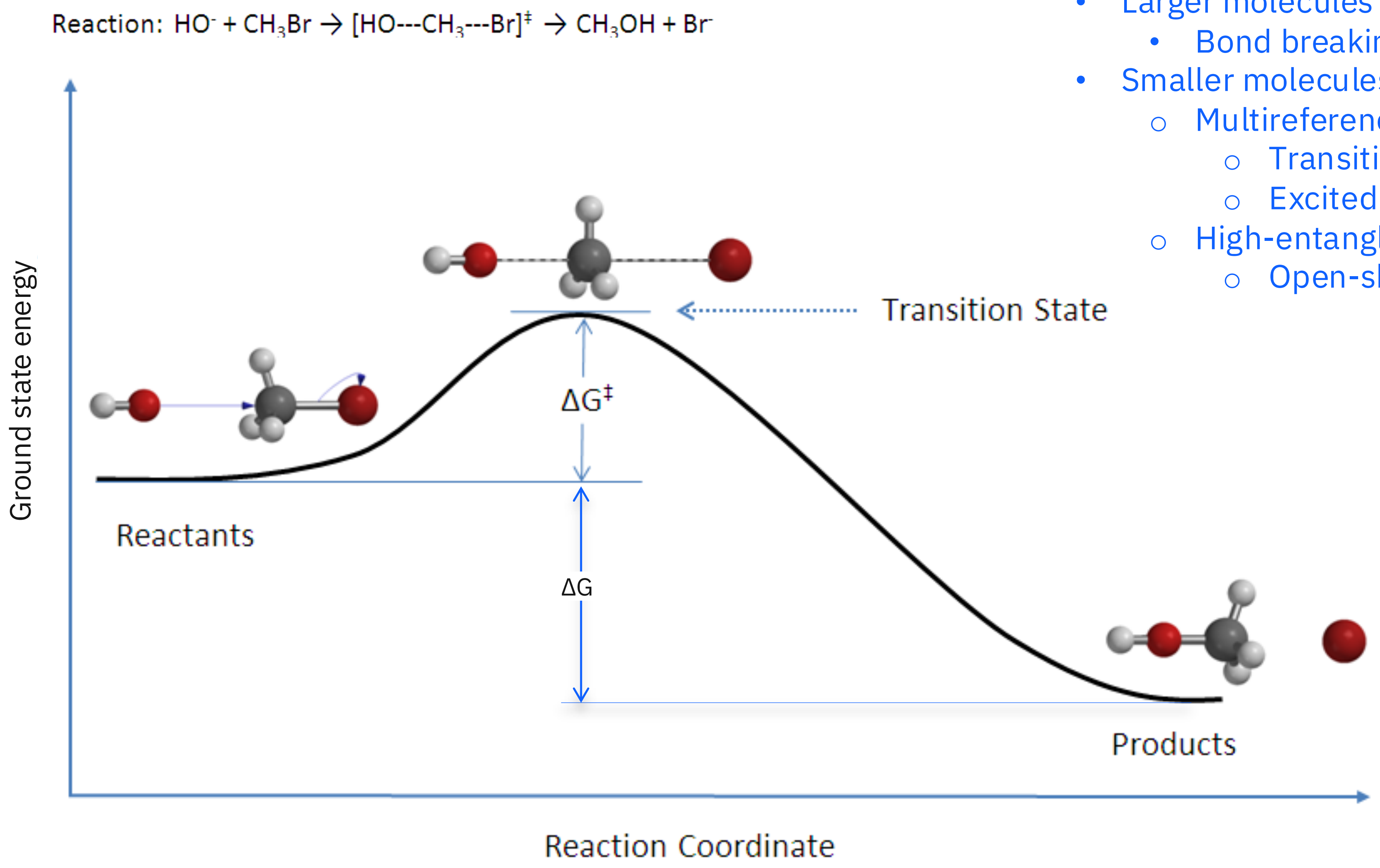
Typical time from material identified in the laboratory to commercialization.

New material process development is constrained by a labor-intensive and time-consuming, trial and error process that must pass through multiple steps, i.e., new materials identification, process development, device development, and product qualification.

[*Materials Genome Initiative | WWW.MGI.GOV*](https://www.mgi.gov)

Why can't classical computers model these use cases?

Example: reaction rates



Challenging for classical computers:

- Larger molecules
    - Bond breaking & formation
- Smaller molecules with
    - Multireference character
        - Transition metals
        - Excited states
    - High-entanglement
        - Open-shell systems

Shor’s Algorithm

Shor's Algorithm is a **quantum algorithm** that can **factor large numbers efficiently**—something classical computers struggle to do.

It threatens RSA encryption, which relies on the difficulty of factoring large numbers. Shor’s algorithm can break RSA in polynomial time using a quantum computer.

Learning

Cat

The limit of bits

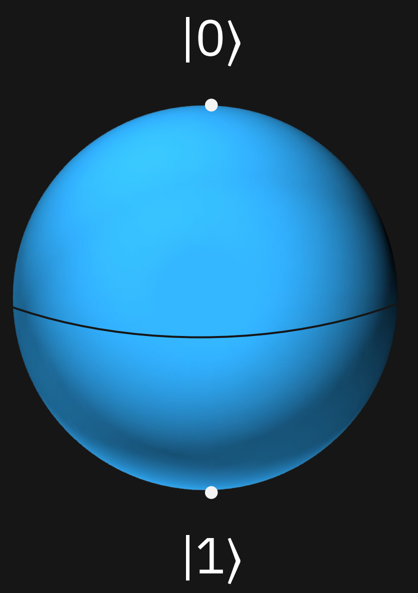
For decades we’ve been simplifying nature into **1**s and **0**s because that was the only way we could manage to create a useful and scalable system of computation.

0010011011100100100010010010011001001110010111
0011111001010010001110001000100101000100100101
0101001010101110010011011100100100010010010011
0010011100101110011111001010010001110001000100
1010001001001010101001010101110111001110010101
1110

But the future isn’t just **1**s and **0**s.

Quantum bits (qubits)

IBM **Quantum**



A quantum bit or qubit is a controllable quantum object that is the unit of information

Quantum processing units (QPUs)

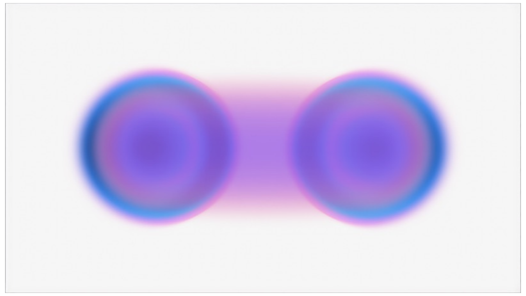
- Apply principles of quantum mechanics
- Qubits can be in more states than 0 and 1
- Use new computational paradigm to obtain answers to previously intractable problems
- Error mitigation lets us run larger, longer circuits
- Computational advantages expected in simulations, search and optimization, and processing data with complex structure

Uniquely quantum

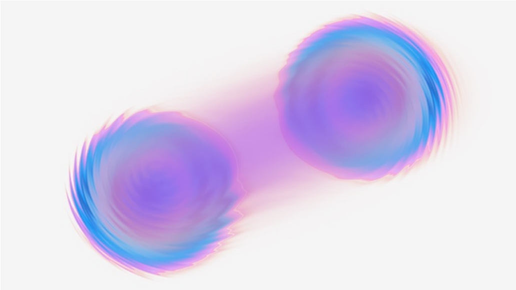
Some problems are classically intractable and will never be solvable with traditional computers

N qubits → 2^N bits
127 qubits → 2^{127} bits = 1.7×10^{38} bits

Superposition
Probabilistic representation of both 0/1 simultaneously



Entanglement
Information shared jointly between entangled pairs or groups



Interference
Interaction that affects likelihood of solutions

Moore's law: the number of transistors in a classical integrated circuit doubles about every two years
... but we are approaching the end due to physical limitations

Approaching the physical limit: IBM created the world's first 2 nm node chip in 2021, with transistors as small as 10 silicon atoms

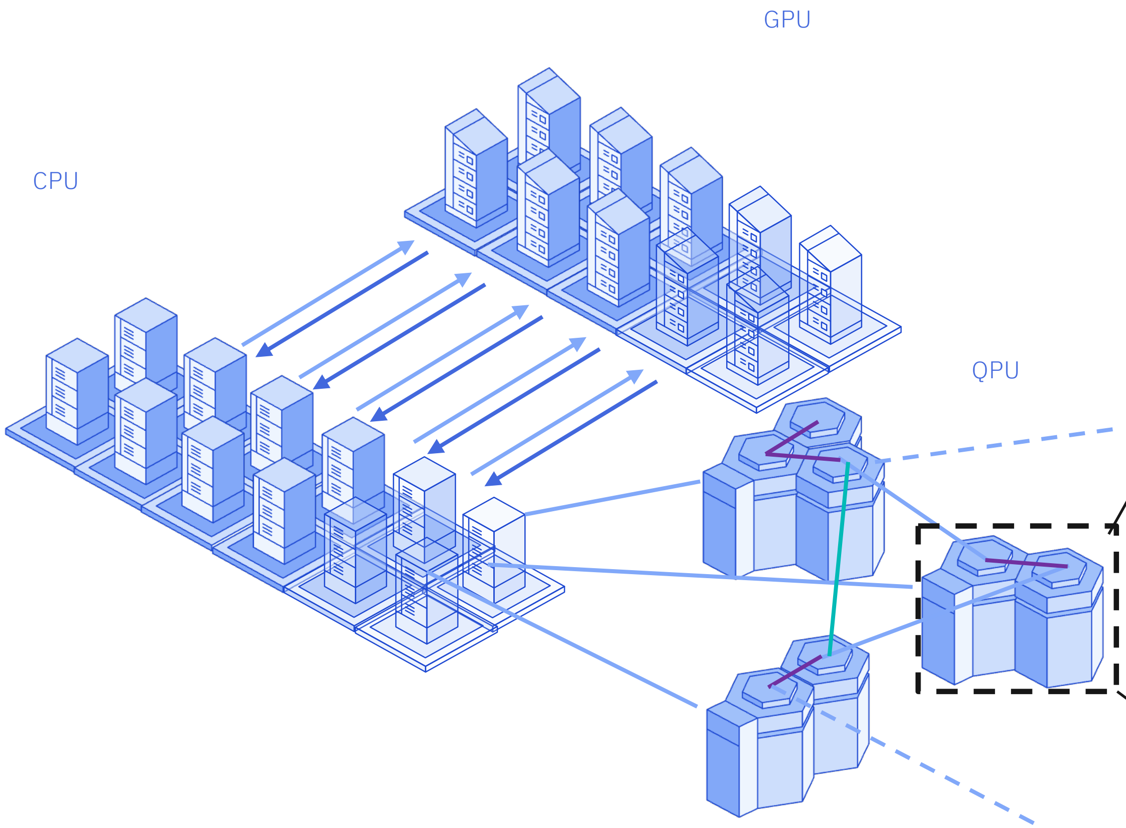
The new wave of computing

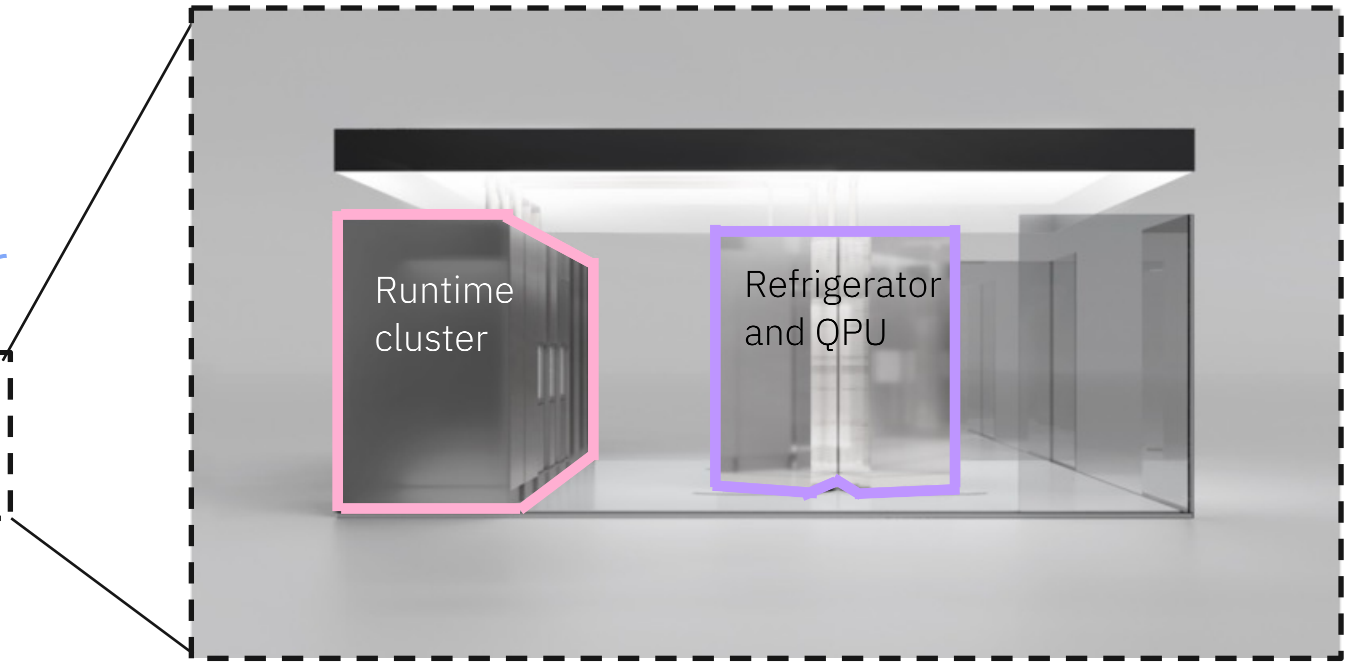
Classical computer
Well suited for many problems.

Quantum computer
Unlock classically intractable problems

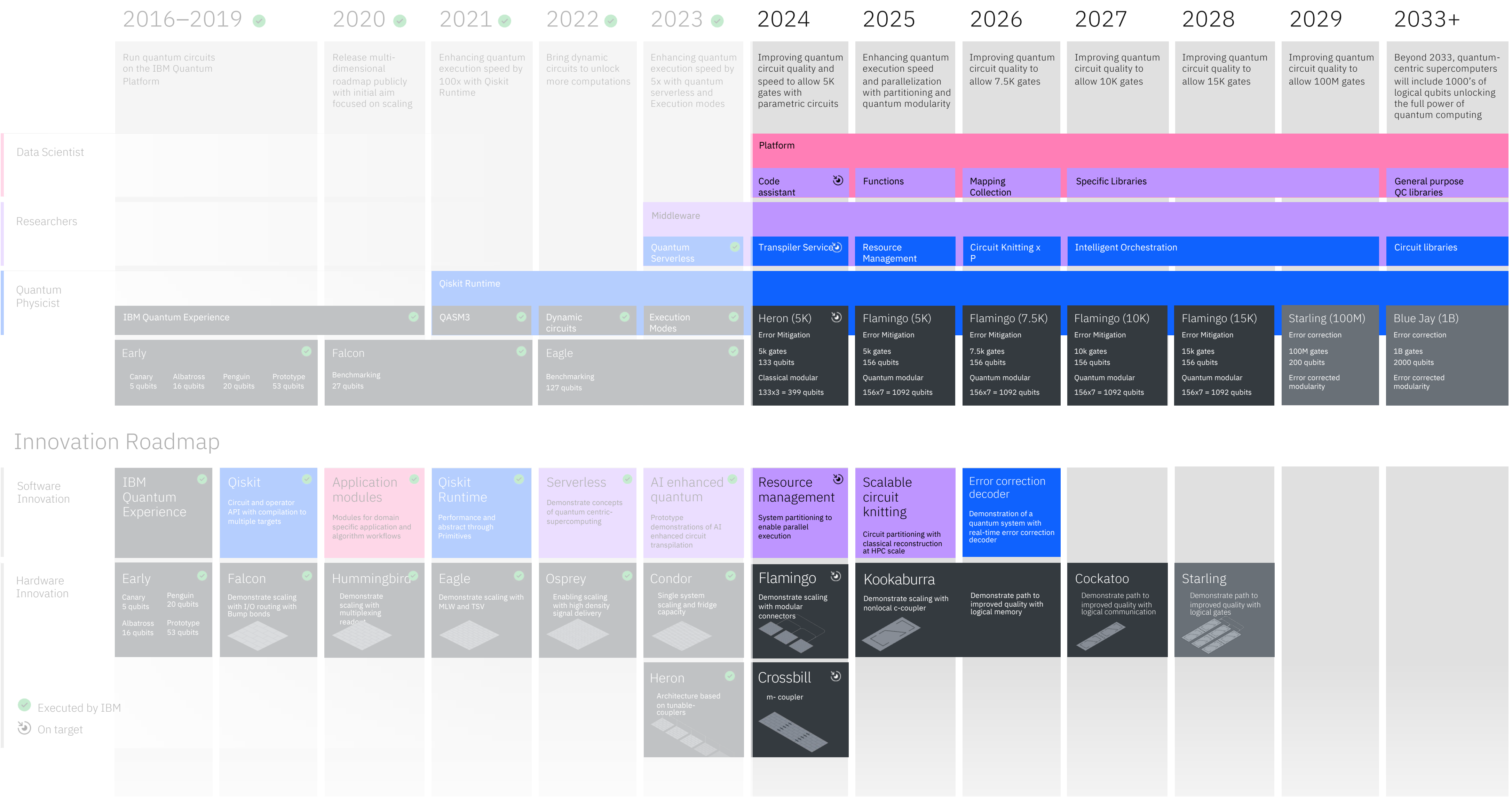
Quantum-centric supercomputing

Delivering impactful quantum computing requires the interplay of quantum and classical resources at scales; quantum-centric supercomputing is the path toward industrial scale applications





Development roadmap



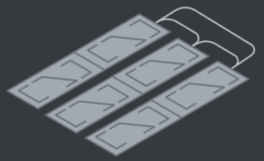
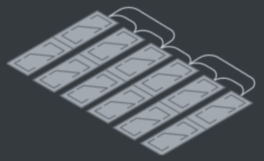
Scaling circuit size through the error correction transition

As we focus on performance, our roadmap highlights a more important metric than qubit count alone: The gate count, which measures the circuit's complexity. We calculate it by multiplying the width—the number of qubits—by the depth, the number of operations you can run on a qubit before it decoheres.

Error mitigation will allow us to increase circuit complexity for the next four years. The tradeoff is that you must run more circuits iteratively and perform classical post processing.

In 2029, we introduce error correction. The width of these circuits—the number of qubits in your calculation—is essentially the same, but you can now run much deeper circuits — those with more operations. The tradeoff is it requires much more physical hardware.

With error correction implemented, we can then start scaling to circuits that are both deeper and wider as we move from Starling to Blue Jay.

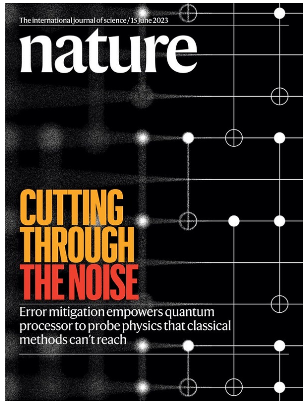
2027	2028	2029	2033+
Flamingo (10K)	Flamingo (15K)	Starling (100M)	Blue Jay (1B)
Error mitigation	Error mitigation	Error correction	Error correction
10k gates 156 qubits	15k gates 156 qubits	100M gates 200 qubits	1B gates 2000 qubits
Quantum modular	Quantum modular	Error corrected modularity	Error corrected modularity
Up to 156x7 = 1092 qubits	Up to 156x7 = 1092 qubits		
			

Theory Utility Advantage

Quantum Utility (2023)

Demonstration that a quantum computer can run quantum circuits beyond the ability of a classical computer simulating a quantum computer

Confirmation via research, papers, & theory



IBM's 2023 research paper ("Evidence for the utility of quantum computing before fault tolerance") provided evidence and methods to move the industry into the Utility era

https://www.nature.com/articles/s41586-023-06096-3

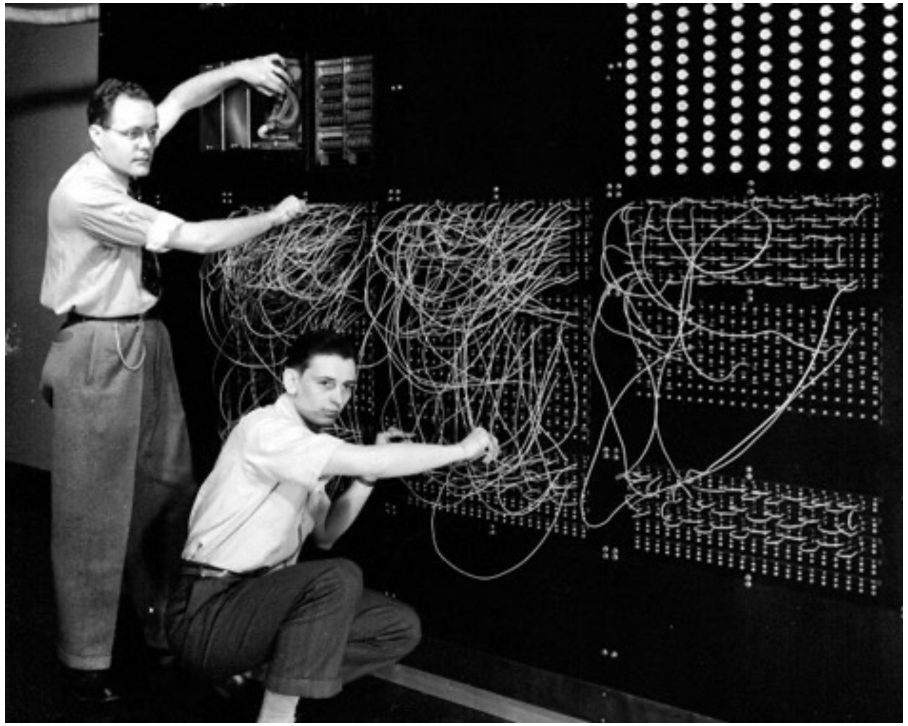
Quantum Advantage (TBD)

Demonstration that a quantum computer can run quantum circuits beyond the ability of all known classical methods

Confirmation via real-world usage

Advantage will come at different times in different domains and depends on the continued advancement of quantum algorithm implementations across industries

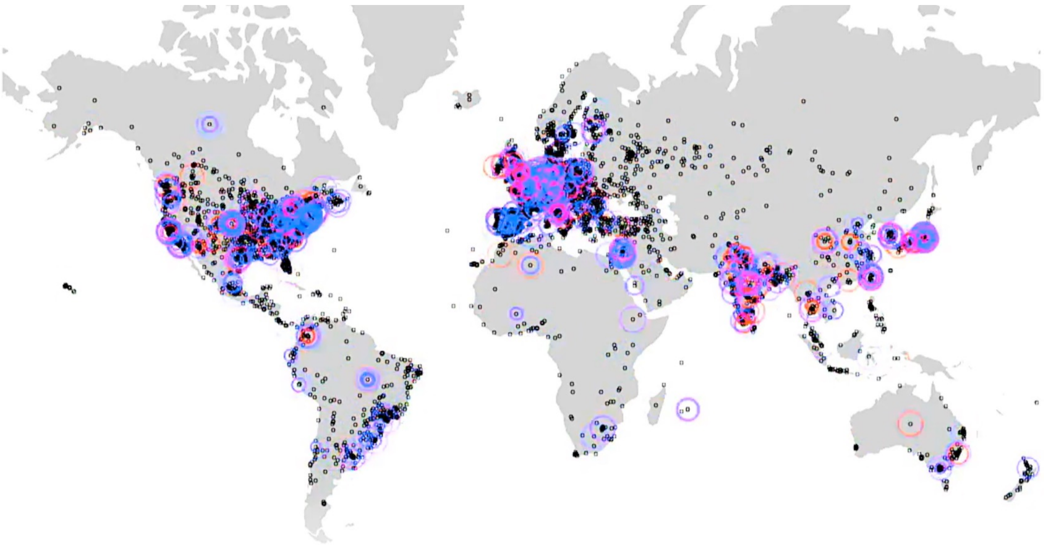
Classical computers before error correction



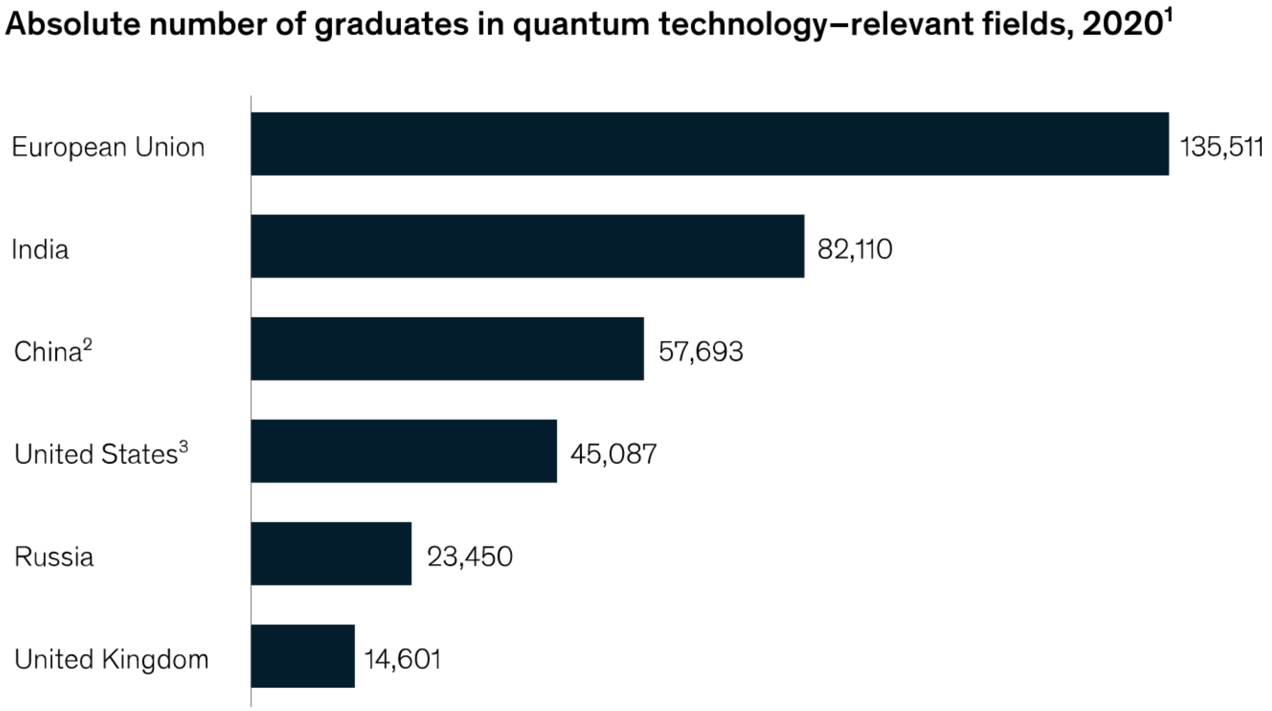
1937	Atanasoff-Berry computer solves systems of linear equations for astronomy research.
1941	British Bombe deciphers German Enigma codes.
1944	IBM Harvard Mark I simulates atomic reactions for Manhattan Project.
1945	ENIAC calculates artillery firing tables for the US Army.
↳ 1950	Hamming “error correction” codes are introduced.

Source: BCG

India’s core strength: Talent



Among the highest users of IBM Quantum Computers



McKinsey Report lists India as having high talent

NQM

विज्ञान एवं प्रौद्योगिकी विभाग
DEPARTMENT OF
SCIENCE & TECHNOLOGY

1. Announced in 2020
2. Cabinet approval in 2023 with budget of Rs 6000 Crores (approx. $ 750 M)
3. Call for preproposals for Quantum Hubs on Jan 20, 2024
4. Preproposals submitted on April 12, 2024
5. Launch of Hubs – Sept 30, 2024

Major role for industry

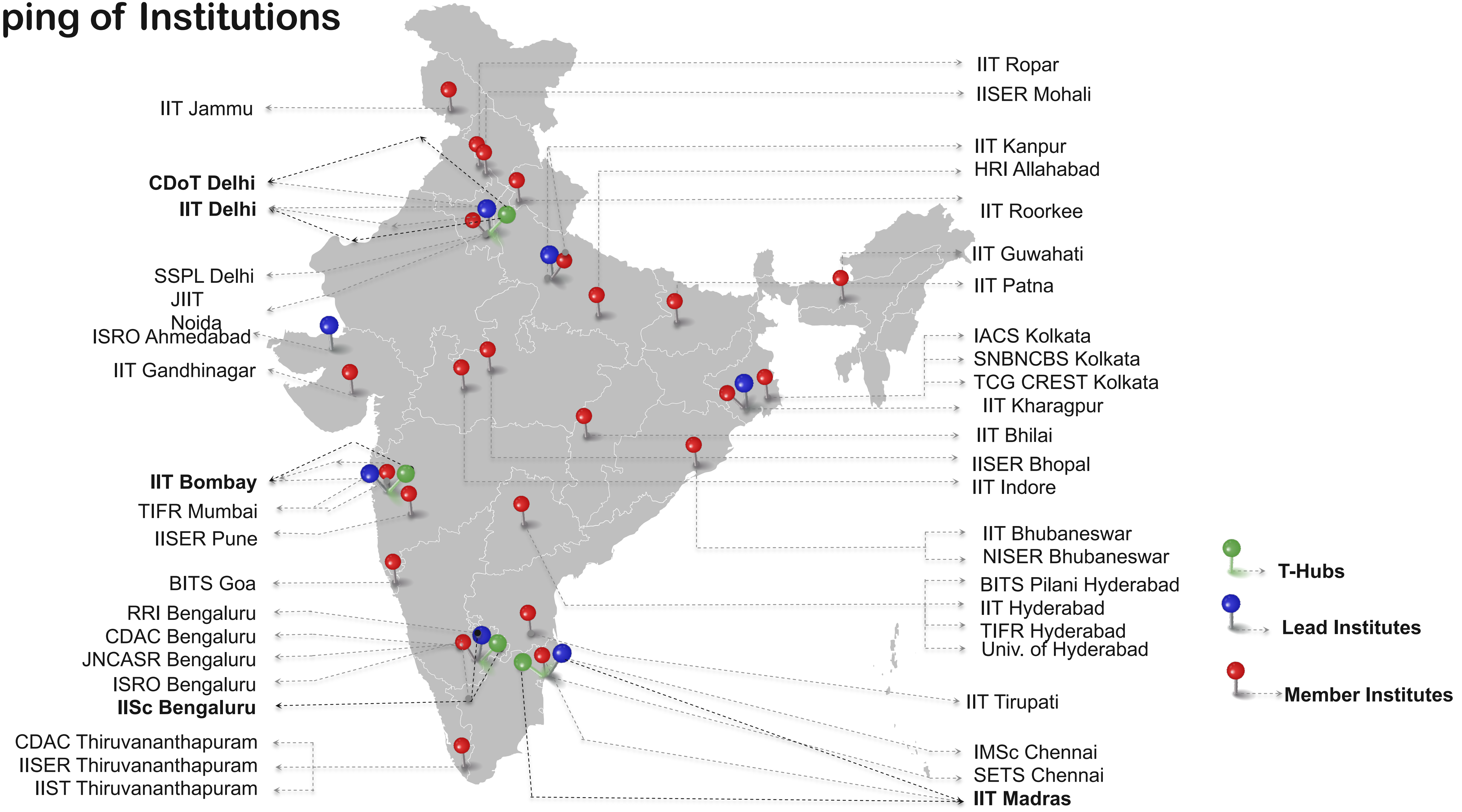
Technology Day Special: Inside India's National Quantum Mission

Rohit Chintapali | May 11, 2024

Technology Day # National Quantum Mission (NQM) # quantum technology # IBM # IIT Madras

The National Quantum Mission (NQM) aims to establish India as a key contender in the global quantum technology landscape, an area where over 30 governments have already pledged more than USD 40 billion in funding across a decade

Mapping of Institutions



- 43 Institutions (Lead & Member) from 17 states and 2 UTs involved in the 17 proposals

India Announces Support For Eight Startups Under National Quantum Mission

Quantum Computing Business   Cierra Choucair • November 26, 2024

6 Courses for a minor program in Quantum Technologies

Open to All Branches

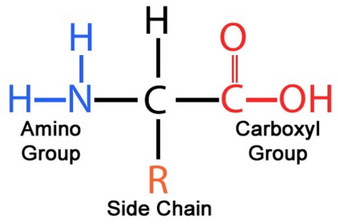
The Indian EXPRESS
JOURNALISM OF COURAGE

AICTE, DST announce UG course in quantum technologies

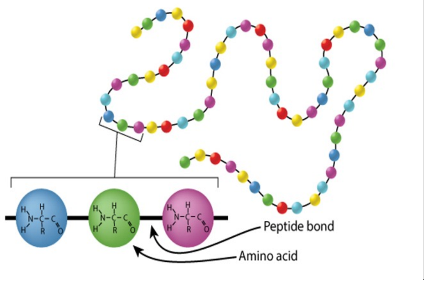
Each course is worth 3 credits, with 1 credit corresponding to 1 hour of in-class instruction per week for a theory course or 1 lab session of 3 hours for a lab course.

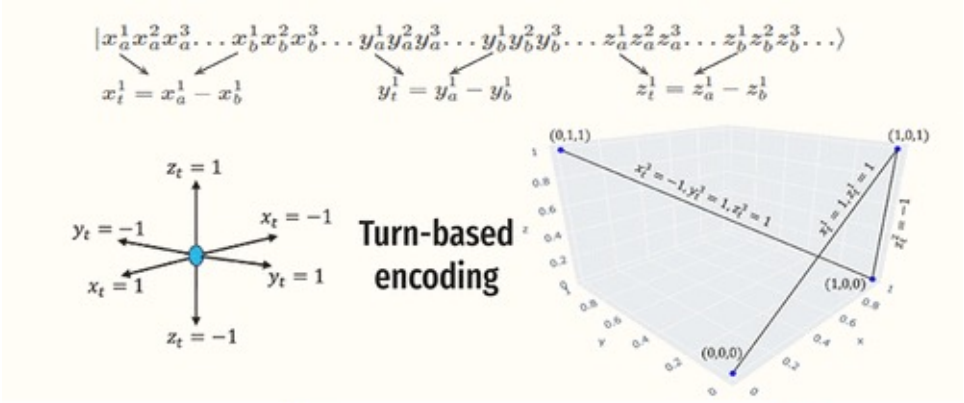
Protein Structure Prediction – IITM + IBM

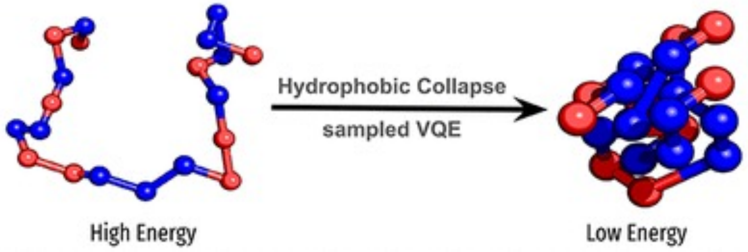
Proteins are biopolymers made up of amino acids



The amino acids are linked by peptide bonds







Journal of Chemical Theory and Computation > Vol 20/Issue 22 > Article

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BIOMOLECULAR SYSTEMS | November 6, 2024

Protein Structure Prediction with High Degrees of Freedom in a Gate-Based Quantum Computer

Jaya Vasavi Pamidimukkala, Soham Bopardikar, Avinash Dakshinamoorthy, Ashwini Kannan, Kalyan Dasgupta*, and Sanjib Senapati*

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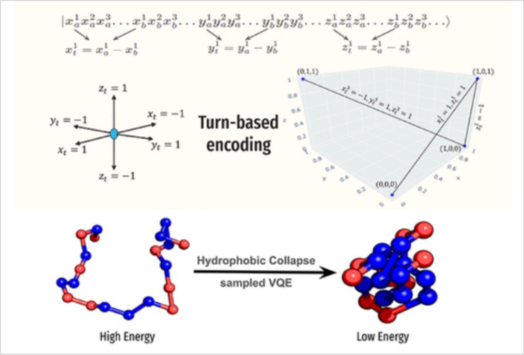
Abstract

Protein folding, which traces the protein three-dimensional (3D) structure from its amino acid sequence, is a half-a-century-old problem in biology. The function of the protein correlates with its structure, emphasizing the need to study protein folding to understand the cellular and molecular processes better. While recent AI-based methods have shown significant success in protein structure prediction, their accuracy diminishes with proteins of low sequence similarity. Classical simulations face challenges in generating extensive conformational samplings. In this work, we develop a novel turn-based encoding algorithm with more significant degrees of freedom that successfully runs on a gate-based quantum computer and predicts



B I G P I C T U R E

114 Qubits

300 two-qubit gates

India's first Utility Scale Experiment

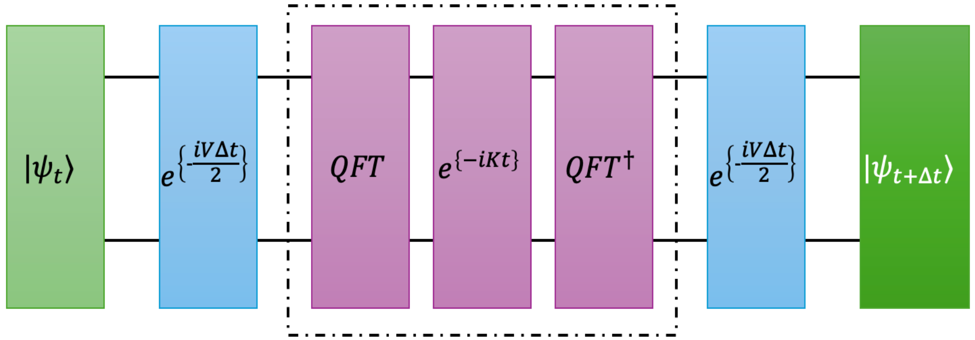
Potential applications

- Protein function prediction
- Drug design and screening
- Identifying protein-protein interactions

Energy Operator Landscapes – Quantum Chemistry GITAM + IBM

Background Theory

- Time evolution operator
- Diagonal Hamiltonian



Existing Algorithm- Complexity

Hadamard basis encoding:

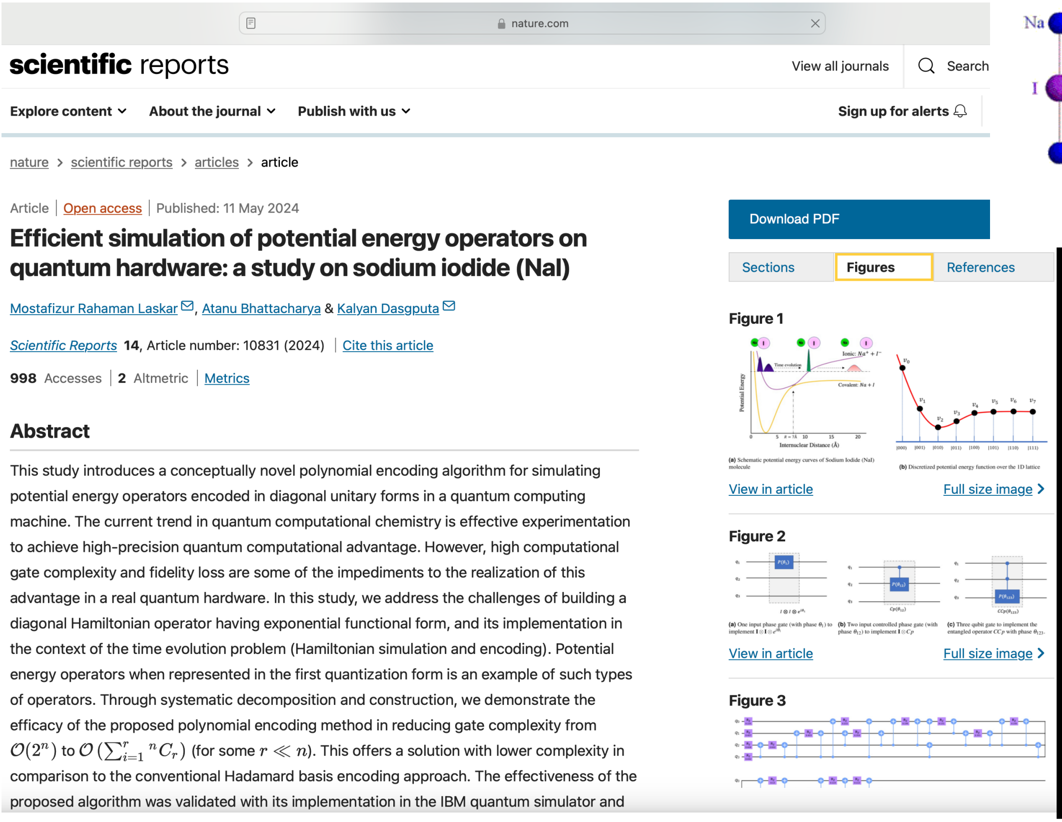
$$n_{CNOT} = \sum_{r=2}^{n} {}^{n}C_r 2(r-1)$$

(Jonathan Welch et. al., Harvard university, 2014, NJP)

Polynomial Encoding (Proposed)

$$\tilde{O}\left(\sum_{j=2}^{r} {}^{n}C_j (2^j - 3)\right)$$

Qubits	Hadamard encoding	2nd order approx	3rd order approx	4th order approx	5th order approx
3	10	3	8	–	–
4	34	6	26	39	–
5	98	10	60	125	154
6	258	15	115	310	484
7	642	21	196	651	1260
8	1538	28	308	1218	2842
9	3586	36	456	2094	5748
10	8194	45	645	3375	10,683
11	18,434	55	880	5170	18,568
12	40,962	66	1166	7601	30,569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Article | Open access | Published: 11 May 2024

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Sections Figures References

Efficient simulation of potential energy operators on quantum hardware: a study on sodium iodide (NaI)

Mostafizur Rahaman Laskar, Atanu Bhattacharya & Kalyan Dasgputa

Scientific Reports 14, Article number: 10831 (2024) | Cite this article

998 Accesses | 2 Altmetric | Metrics

Abstract

This study introduces a conceptually novel polynomial encoding algorithm for simulating potential energy operators encoded in diagonal unitary forms in a quantum computing machine. The current trend in quantum computational chemistry is effective experimentation to achieve high-precision quantum computational advantage. However, high computational gate complexity and fidelity loss are some of the impediments to the realization of this advantage in a real quantum hardware. In this study, we address the challenges of building a diagonal Hamiltonian operator having exponential functional form, and its implementation in the context of the time evolution problem (Hamiltonian simulation and encoding). Potential energy operators when represented in the first quantization form is an example of such types of operators. Through systematic decomposition and construction, we demonstrate the efficacy of the proposed polynomial encoding method in reducing gate complexity from $\mathcal{O}(2^n)$ to $\mathcal{O}(\sum_{i=1}^{r} {}^{n}C_r)$ (for some $r \ll n$). This offers a solution with lower complexity in comparison to the conventional Hadamard basis encoding approach. The effectiveness of the proposed algorithm was validated with its implementation in the IBM quantum simulator and

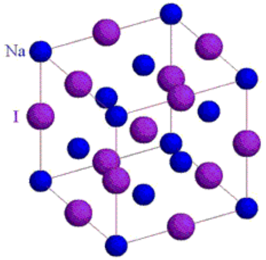
Figure 1

View in article Full size image

Figure 2

View in article Full size image

Figure 3



B I G P I C T U R E

Spec. for QISKIT integration

Experiments: ibmq_mumbai, ibm_Nairobi, simulators

Circuit: 10 Qubits, and 10K shots

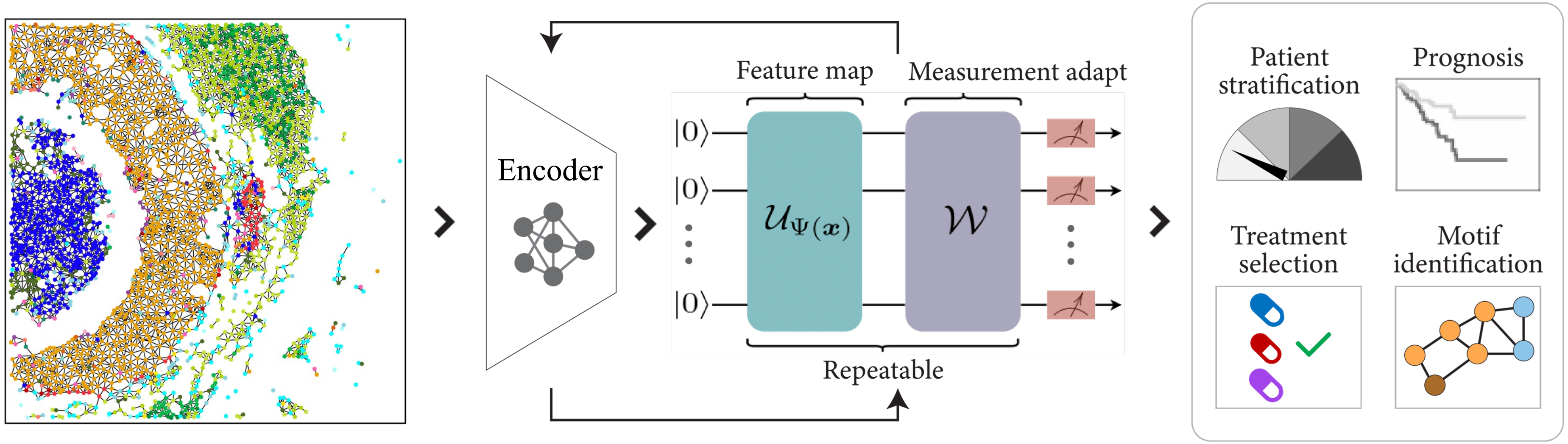
Scalable?

- **Yes**

Potential applications

- Study of energy structure problems in chemical reactions
- Chemical industry, bio-chemistry, Study of storage cells
- Theory can be applied to other domains for 1D functional encoding.

WS2: Spatial Tissue Modeling with Quantum Geometric ML

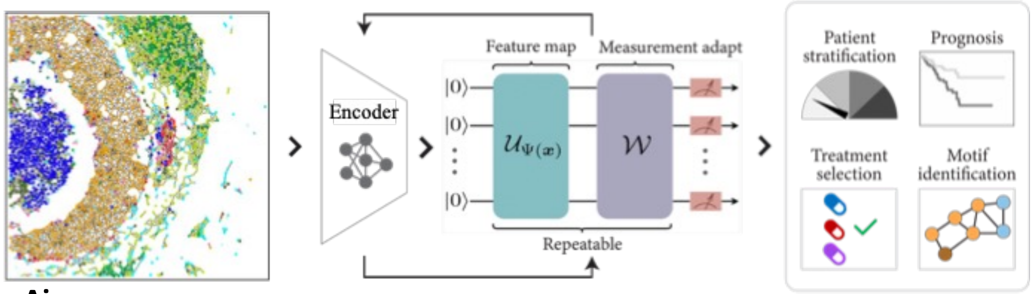


Input:
Spatial tissue graph

Aim:
End-to-end trainable hybrid quantum-classical model:
to learn spatial relationships, contextualize node and graph representation

Target:
- Classification performance
- Motif identification

WS2: Spatial Tissue Modeling with Quantum Geometric ML



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End-to-end trainable hybrid quantum-classical model:
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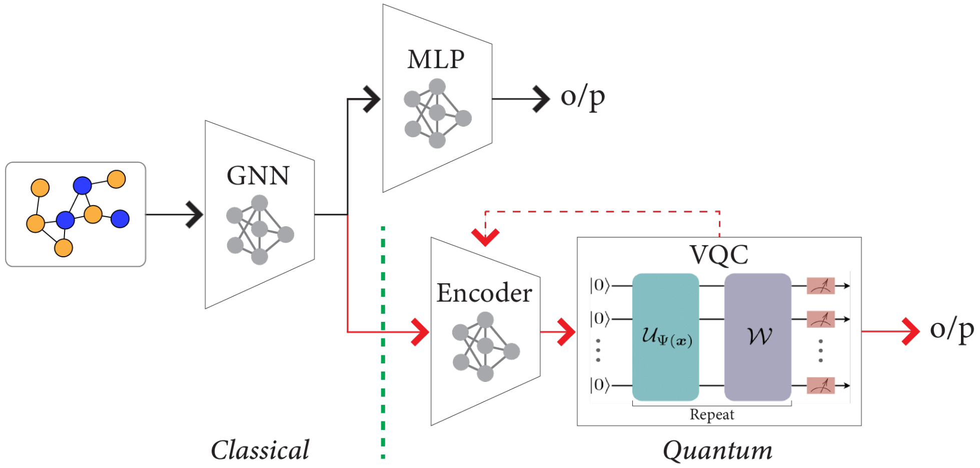
I. Hybrid quantum-classical model: GNN+VQC



GNN- classical Graph Neural Network (GNN) [1]

VQC - Variational Quantum Classifier

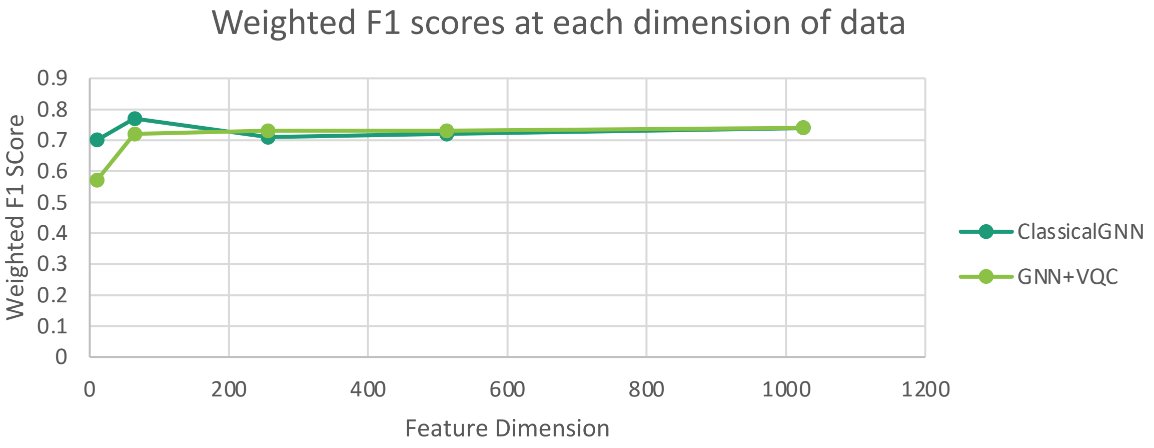


Figure1: Graph showing performance (weighted F1-score) of classical GNN and hybrid quantum-classical model on different feature dimensions.

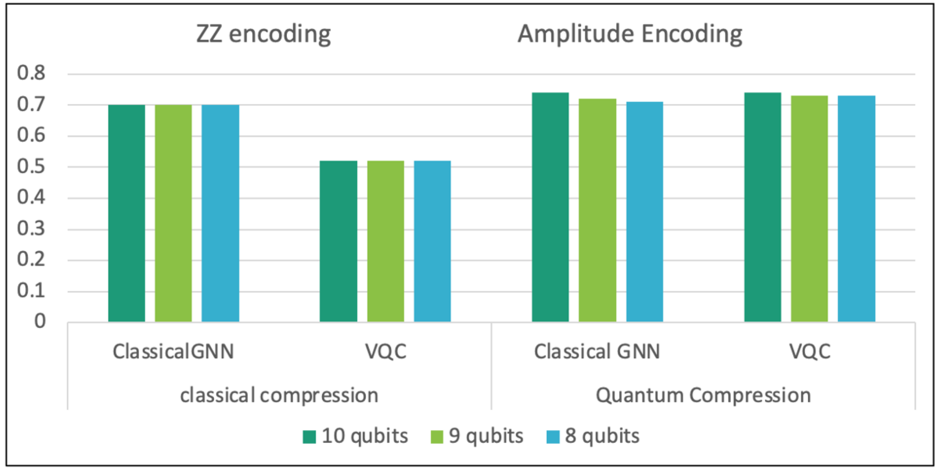


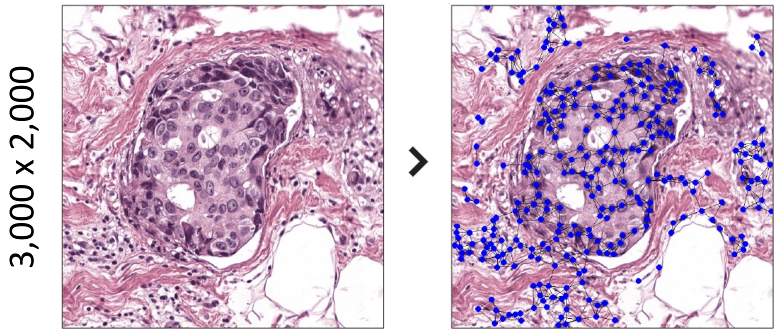
Figure 2: Graph showing efficient training of quantum algorithms via quantum compression instead of lossy classical compression.

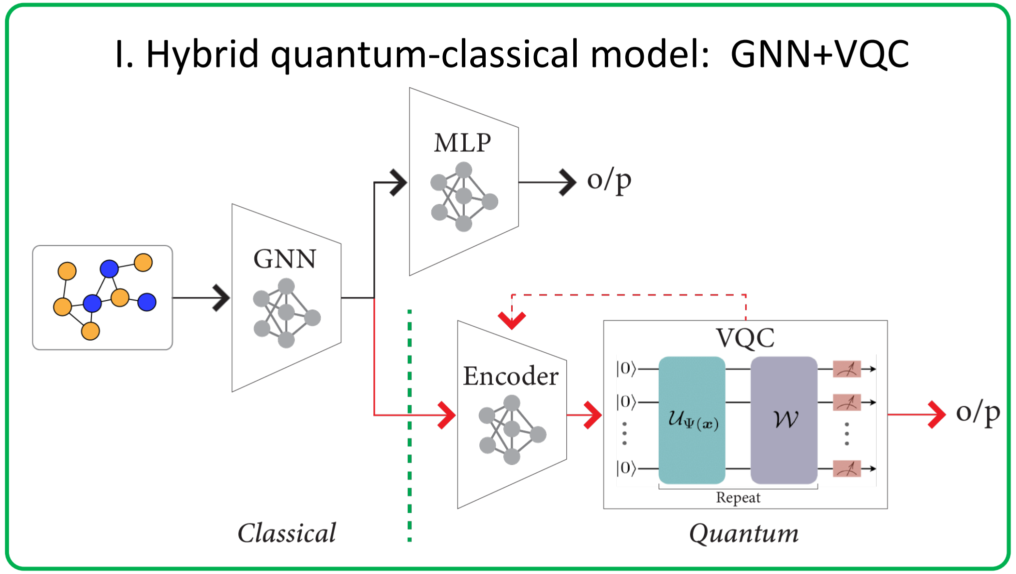
[1] Pati et al., Hierarchical Graph Representations in Digital Pathology, Medical Image Analysis, 2022

IBM Research

WS2: Spatial Tissue Modeling with Quantum Geometric ML

Task 1: Breast Cancer Sub-typing (4 binary classification tasks)





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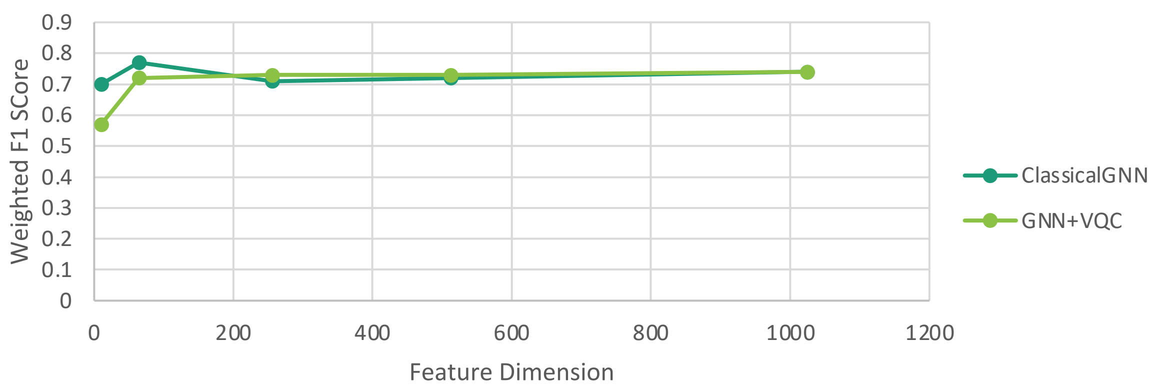
VQC - Variational Quantum Classifier



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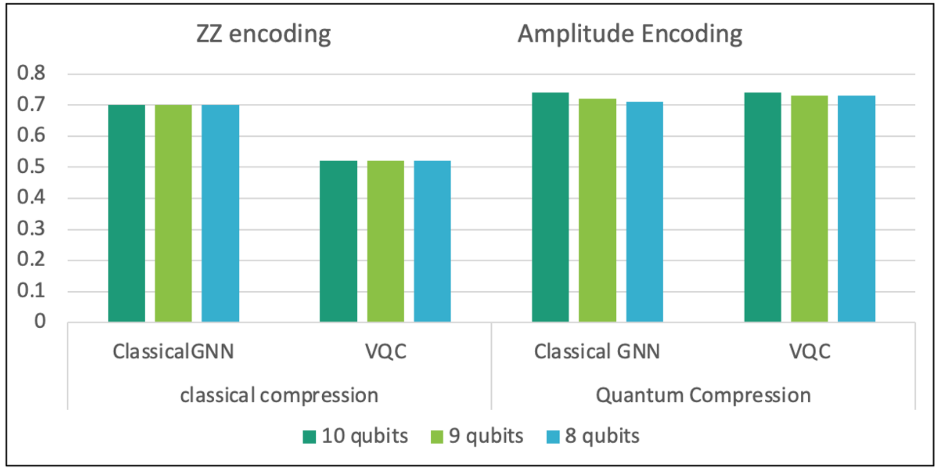

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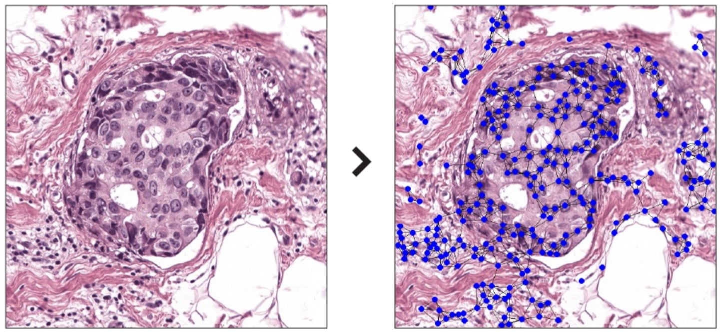
Task 1: Breast Cancer Sub-typing (4 binary classification tasks)

3,000 x 2,000



HYBRID QUANTUM-CLASSICAL GRAPH NEURAL NETWORKS FOR TUMOR CLASSIFICATION IN DIGITAL PATHOLOGY

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[1] IBM Quantum IBM Research India, [2]IBM Research Zurich
[3]Indian Institute of Science Education and Research Tirupati, India

ABSTRACT

Advances in classical machine learning and single-cell technologies have paved the way to understand interactions between disease cells and tumor microenvironments to acceler-

in histopathology [5, 12]. Indeed, a graph representation is a natural modeling choice for TME as it is a flexible data structure to comprehensively encode the tissue composition in terms of biologically meaningful entities, such as cells, tissues, and their interactions. In a typical cell-graph repre-

End-to-end trainable quantum-classical model

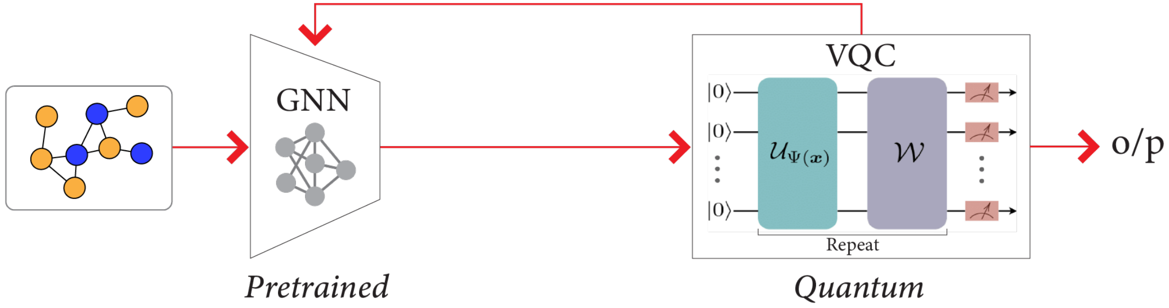

Table 1. Table comparing end-to-end trainable networks vs classicalGNN and classicalGNN+VQC trained separately. All experiments on 10-dimensional ZZ encoding using 10 qubits on the simulator.

Model	w-precision	w-Recall	w-F1score
cGNN	0.71	0.69	0.7
cGNN+VQC	0.58	0.57	0.57
end-to-end GNN+VQC	0.72	0.71	0.72
cSVM	0.68	0.69	0.68
QSVM	0.66	0.68	0.67

GNN- classical Graph Neural Network (GNN) [1]

VQC - Variational Quantum Classifier

[1] Pati et al., Hierarchical Graph Representations in Digital Pathology, Medical Image Analysis, 2022

WS2: Spatial Tissue Modeling with Quantum Geometric ML

- ✓ **PoC**: Hybrid GNN + VQC for breast cancer subtyping:
    - ✓ Serial training of GNN → VQC is on par with classical GNN, amplitude encoding attains better performance than using classical compression
    - ✓ End-to-end training significantly improves over serial training, and even slightly outperforms classical GNN.
- ✓ Paper **in revision to ICASSP '24**: *Hybrid quantum-classical graph neural networks for tumor classification in digital pathology (https://arxiv.org/abs/2310.11353)*
- ✓ Exploring better ansatz design using classical reinforcement learning.

HYBRID QUANTUM-CLASSICAL GRAPH NEURAL NETWORKS FOR TUMOR CLASSIFICATION IN DIGITAL PATHOLOGY

Anupama Ray[1] *Dhiraj Madan*[1] *Srushti Patil*[3] *Maria Anna Rapsomaniki*[2] *Pushpak Pati*[2]

[1] IBM Quantum IBM Research India, [2]IBM Research Zurich
[3]Indian Institute of Science Education and Research Tirupati, India

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Next steps:

- ❑ How to scale the experiments on real hardware ?
- ❑ Can we use a fully quantum GNN for these tasks?

These 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

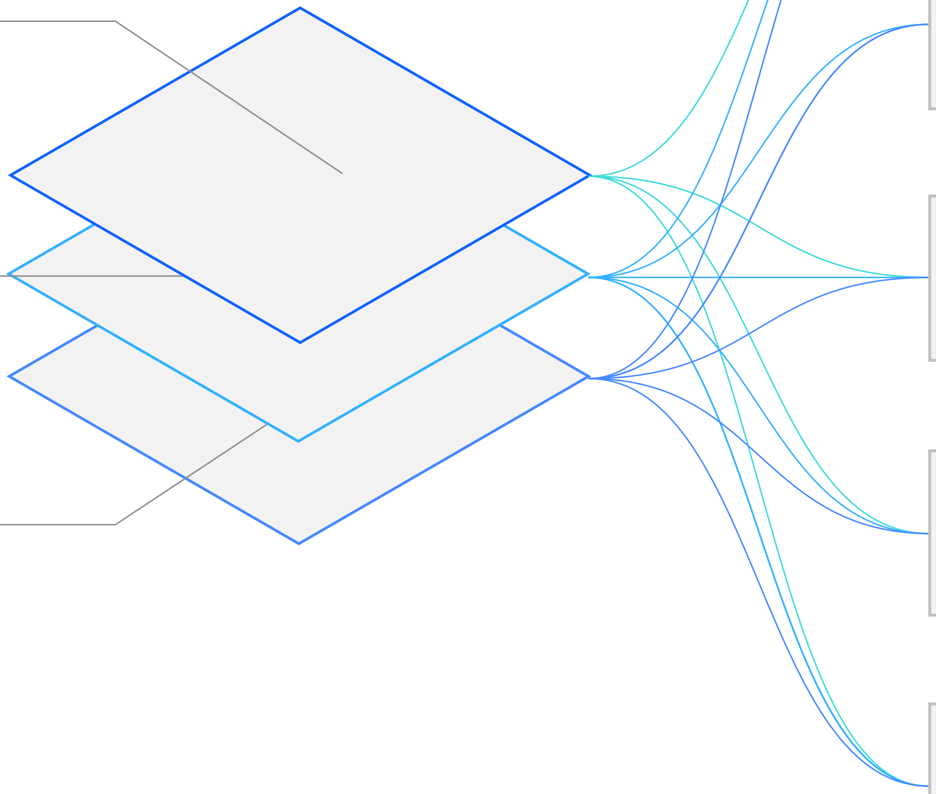
- Network optimization
- Network anomaly detection
- Contextual customer segmentation
- Cybersecurity network

Quantum computing is expected to have impact across industries

Simulating nature

Mathematics and processing data with complex structure

Search and optimization



Aerospace & Automotive

- Customer Experience
- Materials Design
- Structural Design Optimization
- And more

Financial Services

- Fraud Detection
- Derivatives/options pricing
- Portfolio optimization
- Risk analysis
- And more

High Tech

- Seismic Imaging
- Catalysts
- Supply chain planning
- Manufacturing scheduling
- And more

Energy, Environment, Utilities

- Portfolio optimization
- Grid optimization
- Risk Analysis and Options Pricing
- Battery Design
- And more

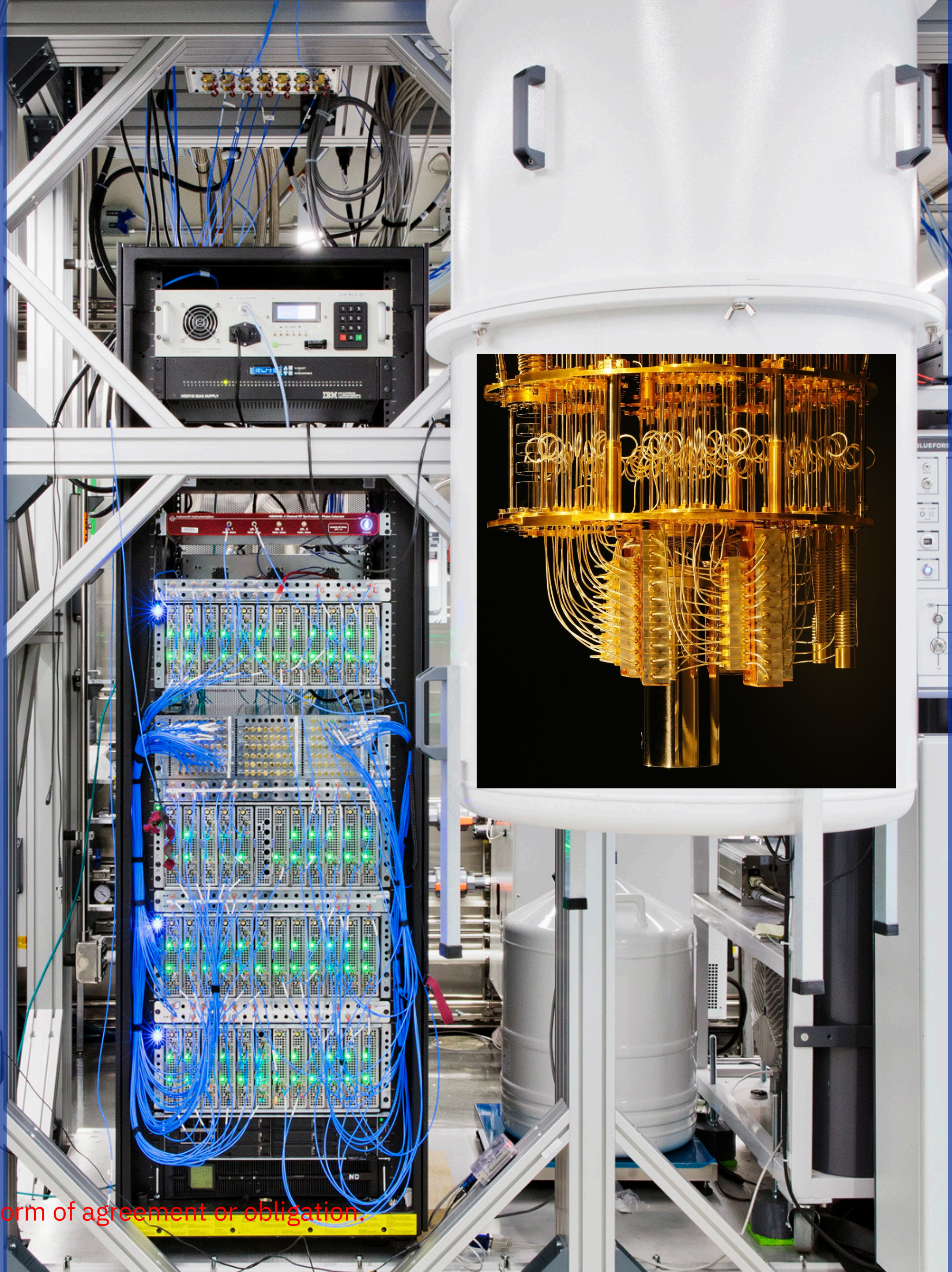
Health Care & Life Sciences

- Disease risk prediction
- Drug discovery and design
- Protein folding predictions
- And more

Global PC Supply Chain

Country	Why It's Crucial
🇨🇳 **China**	Controls **PC manufacturing & final assembly**, largest rare earth supplier
🇺🇸 **USA**	Dominates **chip design, software, and cloud infrastructure**
🇹🇼 **Taiwan**	World's top chip foundry (**TSMC**), critical for all CPUs/GPUs
🇰🇷 **South Korea**	Dominates **memory (RAM/SSD)** and **display panels** (Samsung, LG)
🇯🇵 **Japan**	Leader in **materials, optics, and NAND flash** (Sony, Kioxia, Nitto Denko)

IBM **Quantum** Systems



Stable microwave sources

Analog microwave components and signal digitization

FPGA based microwave pulse shaping control units

Thermalization and cryogenic stability

Coaxial cabling for I/O signal integrity

Microwave signal isolators

Cryogenic amplifiers

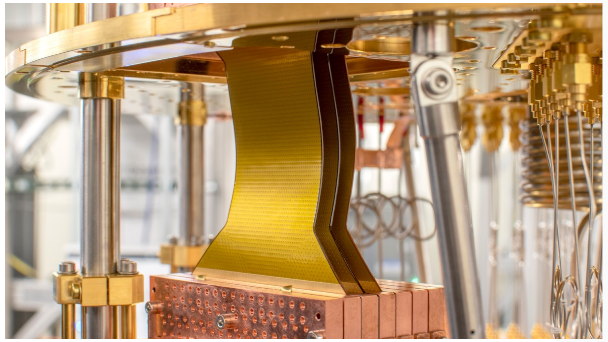
Quantum processor

Component supply chain for quantum

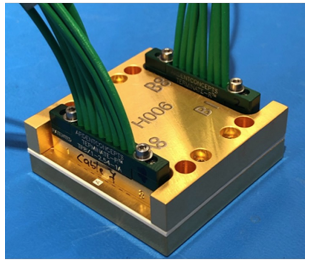
IBM **Quantum**

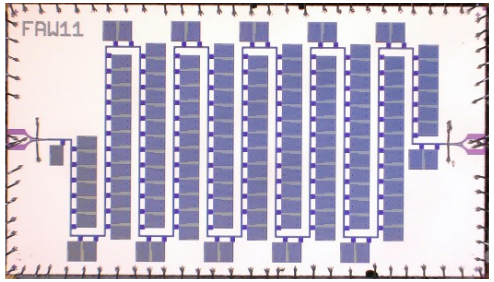
IBM is actively supporting to foster the growth of the supply chain for quantum with global industry players in the areas of **cryogenics, control electronics, quantum communications, and scalable I/O** for a scalable quantum computing systems.

I/O wiring and space transformers

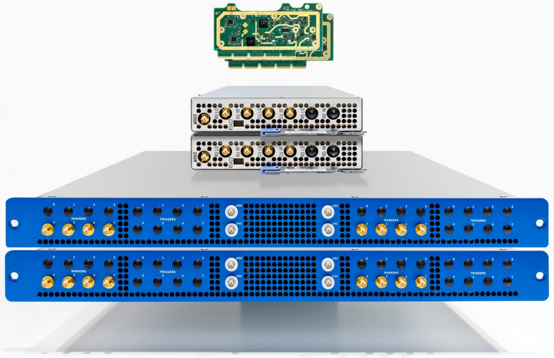


Amplifiers and other microwave components

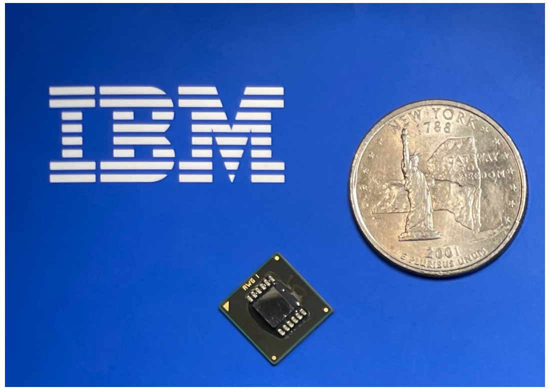




Control electronics



Full-featured 4K cryo-CMOS qubit controller

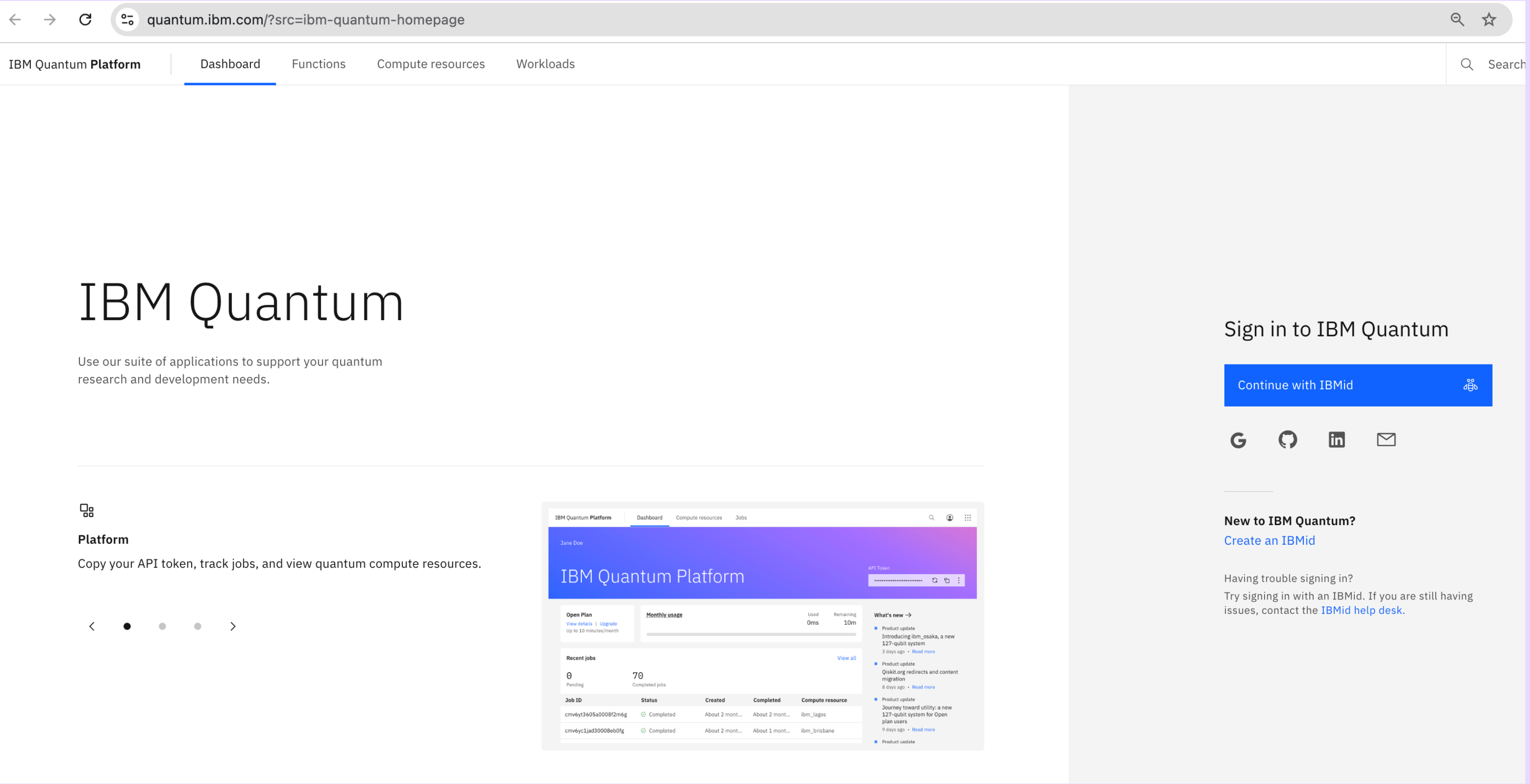


Runtime Infrastructure

Cyro Infrastructure

For discussion purposes only and does not constitute any form of agreement or obligation.

Why now?


quantum.ibm.com/?src=ibm-quantum-homepage
IBM Quantum Platform
Dashboard
Functions
Compute resources
Workloads
Search
IBM Quantum
Use our suite of applications to support your quantum research and development needs.
Platform
Copy your API token, track jobs, and view quantum compute resources.
IBM Quantum Platform
Sign in to IBM Quantum
Continue with IBMid
New to IBM Quantum?
Create an IBMid
Having trouble signing in?
Try signing in with an IBMid. If you are still having issues, contact the IBMid help desk.

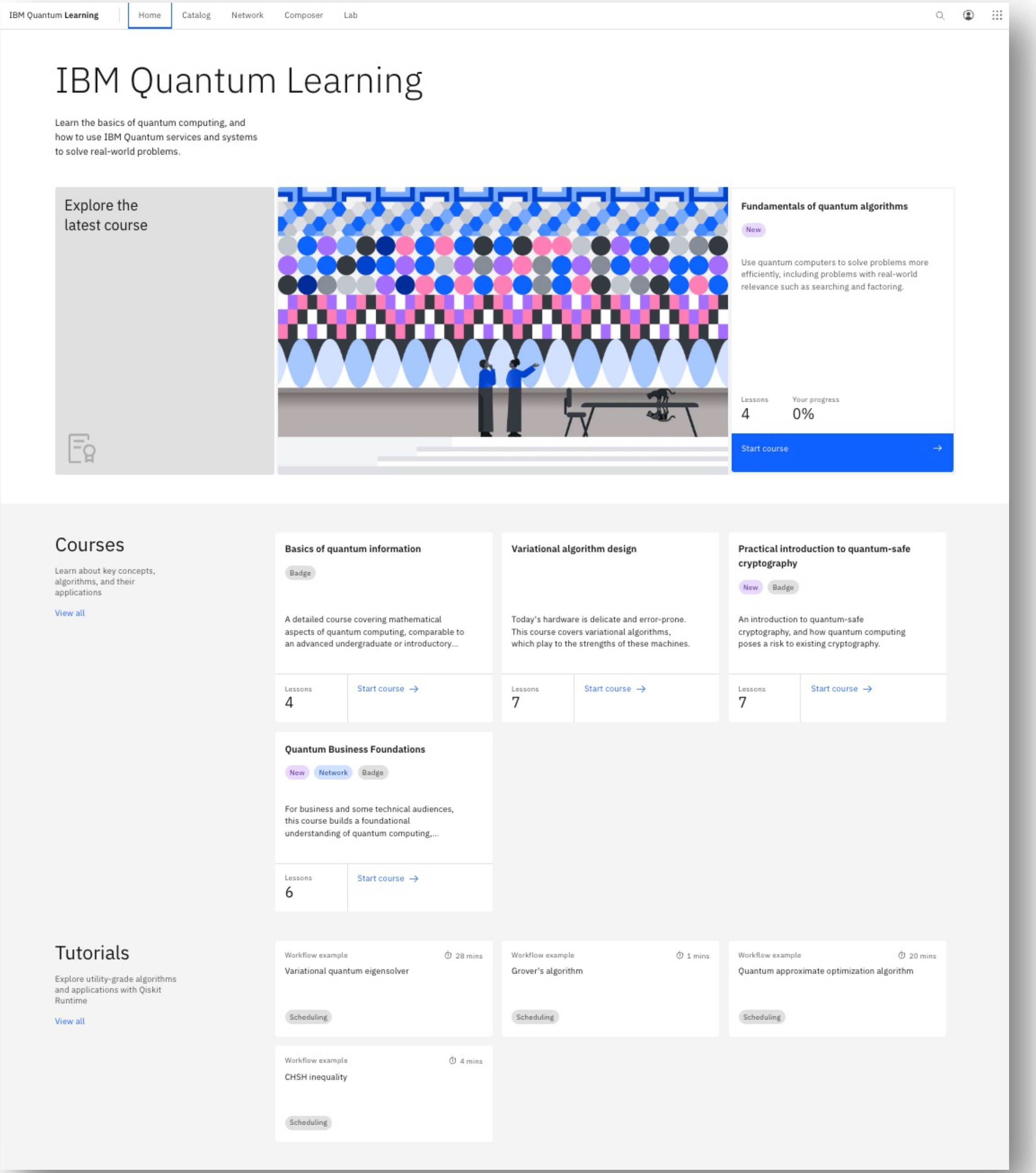
IBM Quantum Learning

Learn the basics of quantum computing and how to solve real-world problems with IBM Quantum services and systems

- Access courses, tutorials, and other learning resources created by leading quantum experts like John Watrous
- Log in to track course progress
- Earn badges for selected courses

Get started today

↓



Mercedes-Benz

Materials discovery and manufacturing optimization

Mercedes-Benz and IBM have published a series of papers demonstrating progress toward using quantum computers to model material systems, including lithium-sulfur, that are relevant to advancing the performance of batteries.

The teams are also exploring applications in manufacturing defect analysis and product recommendation.

- Journal of Chemical Physics 154.13 (2021): 134115.
- Nature 567.7749 (2019): 491-495.
- arXiv:2004.00957

"Developing and perfecting these hypothetical batteries could unlock a billion-dollar opportunity."

Benjamin Boeser
[Former] Director of Innovation Management
Silicon Valley at Mercedes-Benz R&D America

Higher manufacturing uptime

Business imperative

The uptime of the production line is one of the most important metrics in manufacturing. When the production line is interrupted, costs continue to accrue, while product is not produced.

Current state

Fault detection and classification (FDC) suffers from high false positive rates. Data is often difficult, time-consuming, and expensive to obtain. This is particularly true for highly imbalanced datasets, such as FDC, where the ratio of non-faults to faults can exceed 10,000:1.

Business value exploration

Quantum machine learning models have demonstrated higher accuracy on smaller datasets.

Delta Air Lines

Gate scheduling optimization

Optimizing large combinations of cargo and passenger traffic among the planes, gates, personnel, and the air traffic flows originating and terminating at an airport helps airlines to control costs and reduce inefficiencies.

Delta and IBM partnered to explore the application of quantum computing to airline gate-scheduling quadratic assignment problems (QAP).

The team applied the variational quantum eigensolver (VQE) with a new space-efficient quadratic unconstrained binary optimization (QUBO) algorithm that maps a *k*-coloring problem to a lower number of qubits.

https://arxiv.org/abs/2111.09472

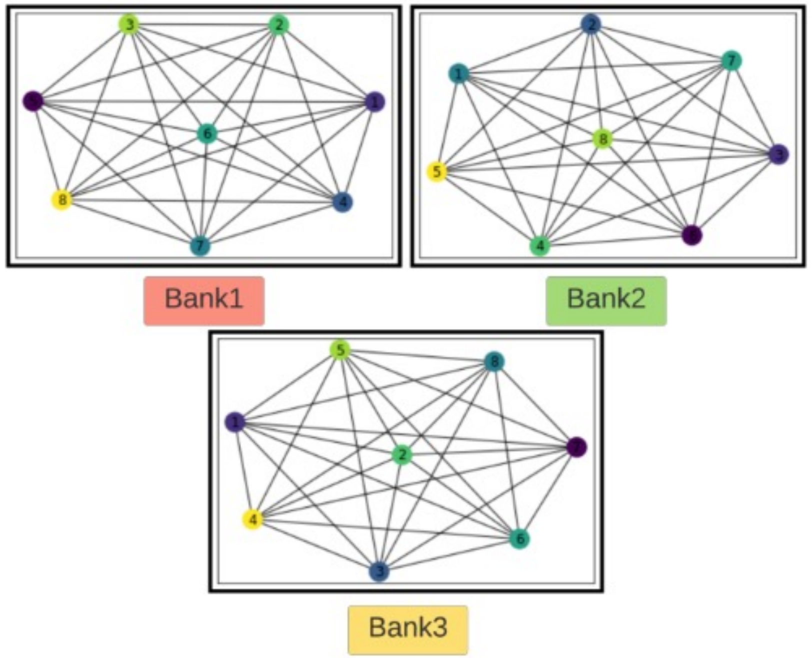


Figure 4 Quantum simulation results for 24 flights and eight gates. The graph successfully colored by the applying the efficient embedding technique.

Table 1 Comparison between the standard QUBO and the efficient embedding approaches

	Standard Embedding	Efficient Embedding
# Qubits	$n \times k$: 25	$n \times log(k)$: 15
Circuit Depth	29	19
Run-time (sec)	5569.84	395.48

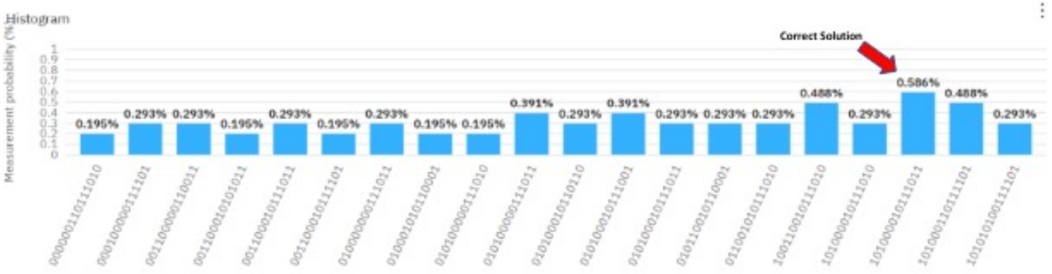


Figure 6 Hardware results with the measurement probabilities for a bank with eight flights and eight gates.

Boeing

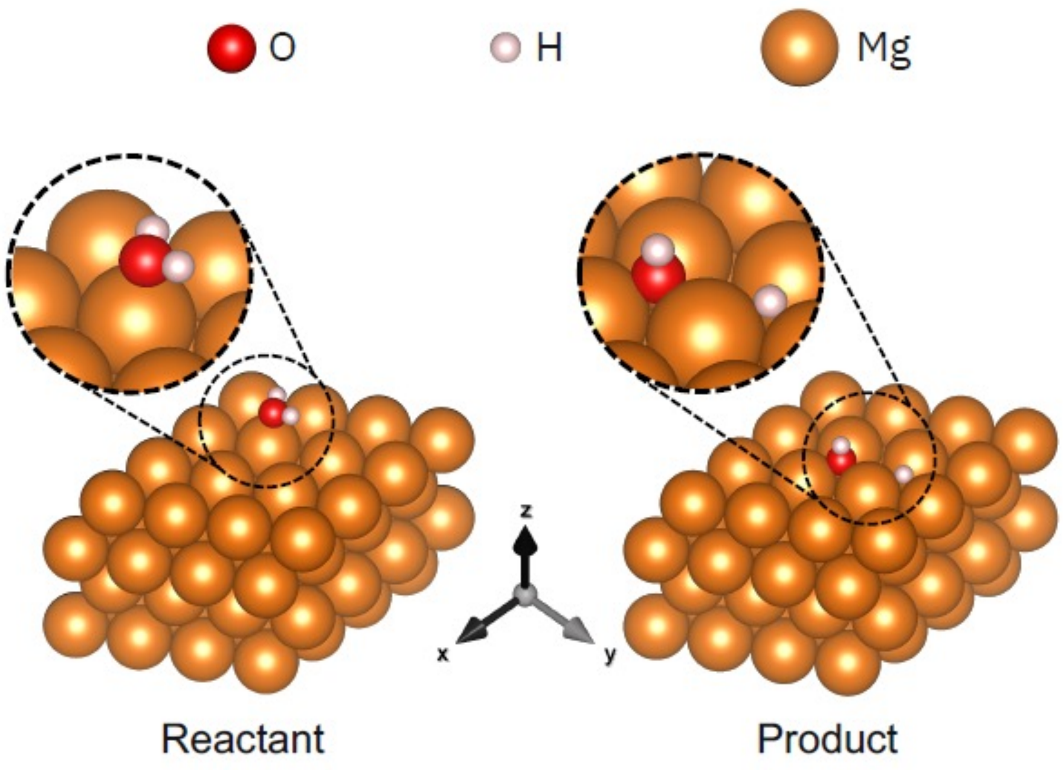
New materials qualification

IBM and Boeing model corrosion reactions for magnesium, the lightest structural metal

Magnesium has the potential to improve the weight of critical aerospace structures. However, magnesium reacts with water and corrodes readily.

IBM simulated the reaction of water with magnesium to better understand its reaction mechanisms to explore the possibility of lighter, higher-performance aerospace structures.

$$Mg + H_2O \rightarrow Mg(OH)_{ads}(H)_{ads}$$



arXiv:2203.07536

Exoplanet discovery

Business imperative
With new and advanced telescopes, data in astronomy is growing at a fast pace. Conventional methods to discover exoplanets that involve human judgment are not efficient and are prone to variability depending on the investigating expert.

Current state
Commonly used data analysis techniques for exoplanet detection with the transition method produce many false positives in the case of noisy data. These false positives must be reviewed manually.

Business value exploration
Quantum machine learning methods may help improve the classification accuracy of exoplanet candidates and reduce the rate of false positives.

Satellite image classification

Business imperative

Earth observation imagery plays numerous crucial roles, such as monitoring agriculture, water management, and climate change.

Current state

Hundreds of terabytes of images are collected daily. Correctly classifying these images is a first step in deriving useful information.

Business value exploration

Quantum computing may enable more accurate satellite image classification, which in turn can allow faster and more accurate management of crucial resources.

ExxonMobil

Routing optimization

In 2021, more than 500 liquified natural gas (LNG) ships were used to transport critical fuel supplies across the oceans. Together, they make thousands of journeys per year to destination ports where the LNG is deployed to power critical infrastructure.

Finding optimal routes for a fleet of such ships can be a mind-bendingly complex optimization problem.

https://www.ibm.com/case-studies/exxonmobil/
https://arxiv.org/abs/2003.02303v2
IEEE Trans Quantum Engineering, vol. 2, p. 1

Quantum computers take a new approach to addressing this sort of complexity, with the potential to find solutions that classical supercomputers alone cannot handle. Industry leaders like ExxonMobil are getting involved now to explore how blending classical and quantum computing techniques might solve big, complex, pressing global challenges.

E.ON

E.ON is partnering with IBM to drive the transformation of the energy industry with quantum computing.

Their goal is to explore the potential of quantum computing to optimize the world's rapidly decentralized energy infrastructure.

Some areas under consideration are whether quantum computing could be used to help control grid-connected renewable energy systems and to optimize electric car charging processes.

Woodside Energy

Since 2019, Woodside Energy has been working with IBM to explore the potential for quantum computing and AI to help realize its vision of an intelligent plant.

"We are deploying advanced technologies to capture, analyse and use all available data as we progress our Burrup Hub growth plans, reducing costs and risk whilst improving reliability and production performance. **The relationship with IBM has been a crucial part of our work in artificial intelligence and will now assist us to build capability in quantum computing."**

Peter Coleman
CEO, Woodside Energy

Fraud Detection

Business imperative

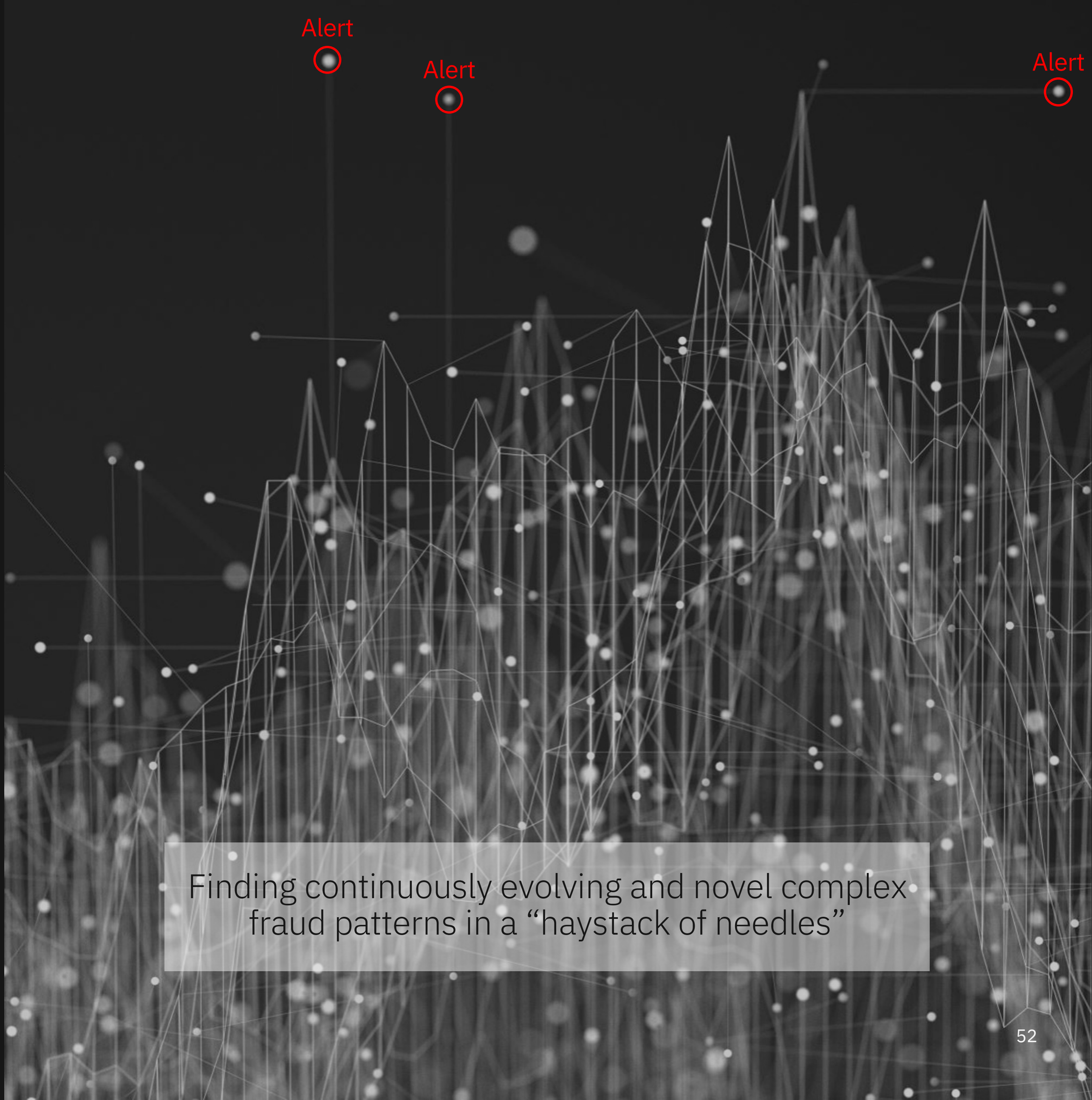
Trust in financial systems relies on effective monitoring and control mechanisms to detect and halt fraudulent activity – or *needles in a haystack*. Thus, financial institutions are required to demonstrate regulatory *effectiveness* of such mechanisms, while *reducing operational cost* that would enable budget allocation to innovation and *improving customer experience* and *attrition due to false positive reduction*.

Current state

Depending on the respective type of fraud and jurisdiction, banks are employing both business rules and state of the art machine learning/AI algorithms, while still having to *strike compromises* between detection rates and false positives, and thus substantial cost for quality assurance of compliance control functions.

Future state

Quantum machine learning algorithms combined with the latest advances in classical AI *improve fraud pattern recognition* due to higher dimensional data embeddings and resolution of statistical imbalances, and thus allowing for more effective monitoring and control mechanisms that free-up compliance officers to focus on more complex cases requiring extra expert knowledge and data.



Brighter, more energy-efficient displays

JSR and Mitsubishi Chemical

- JSR, Mitsubishi, and IBM modeled the electronic structure of OLED molecules that have the potential for **100% internal quantum efficiency**

- Conventional OLED emitters are inherently limited to 25% internal quantum efficiencies

Source: Computational Materials 7.1 (2021): 70.

What is Quantum Advantage?

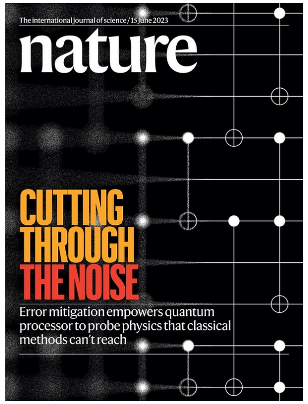
Utility vs. Advantage

Theory | Utility | Advantage

Quantum Utility (2023)

Demonstration that a quantum computer can run quantum circuits beyond the ability of a classical computer simulating a quantum computer

Confirmation via research, papers, & theory



IBM's 2023 research paper ("Evidence for the utility of quantum computing before fault tolerance") provided evidence and methods to move the industry into the Utility era

https://www.nature.com/articles/s41586-023-06096-3

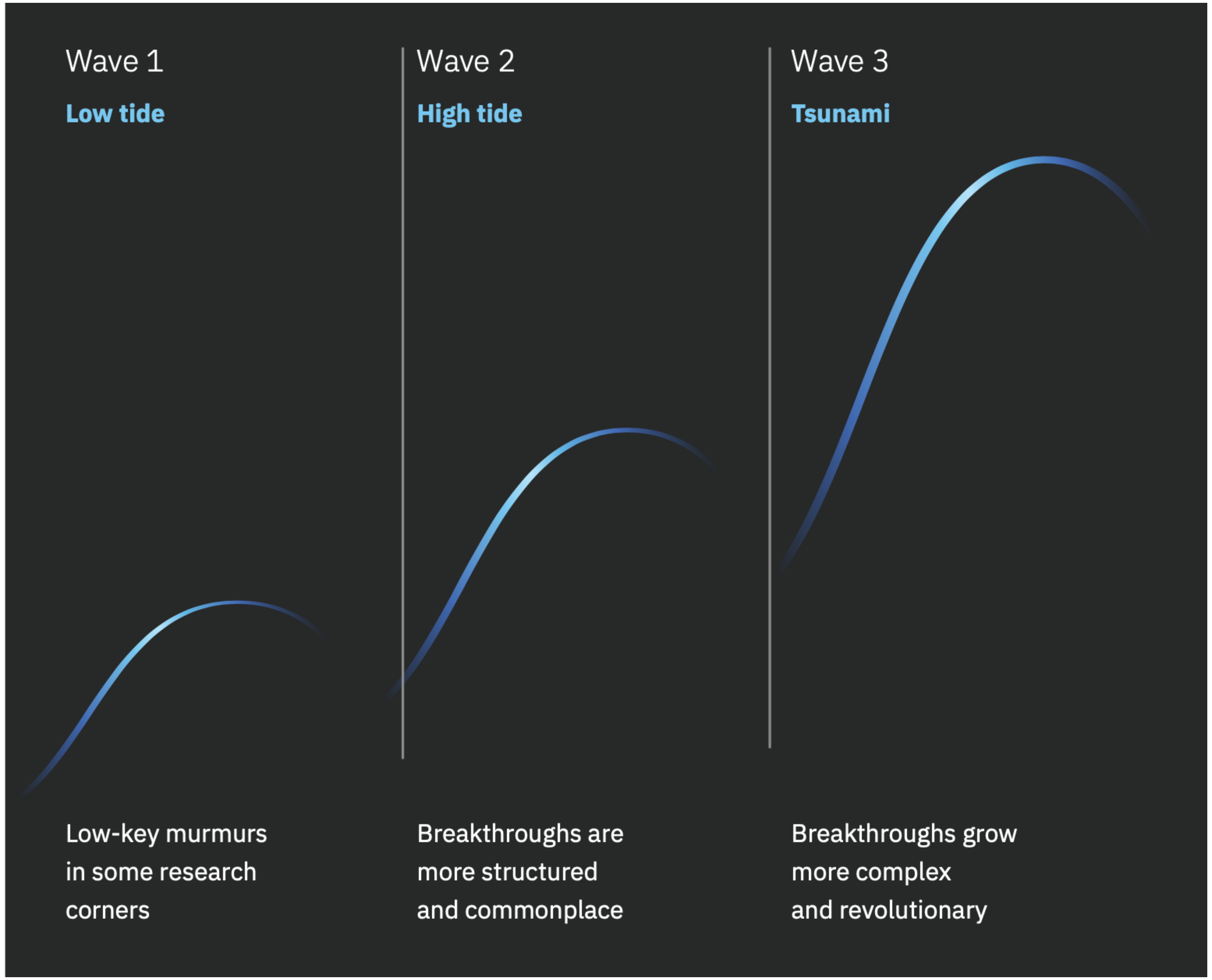
Quantum Advantage (TBD)

Demonstration that a quantum computer can run quantum circuits beyond the ability of all known classical methods

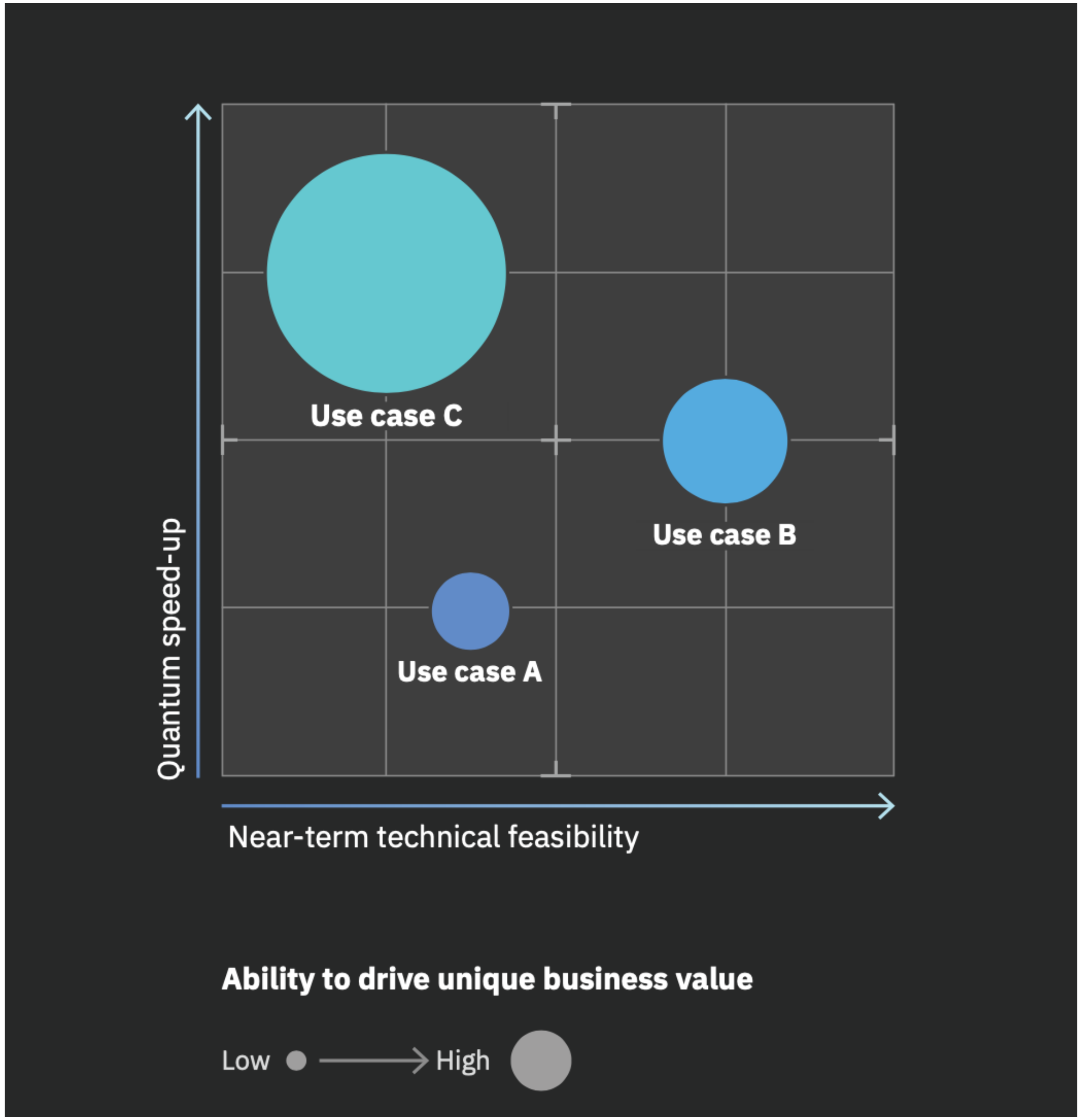
Confirmation via real-world usage

Advantage will come at different times in different domains and depends on the continued advancement of quantum algorithm implementations across industries

The Three waves in the life of key Technologies



Quantum Advantage and the quest for business value

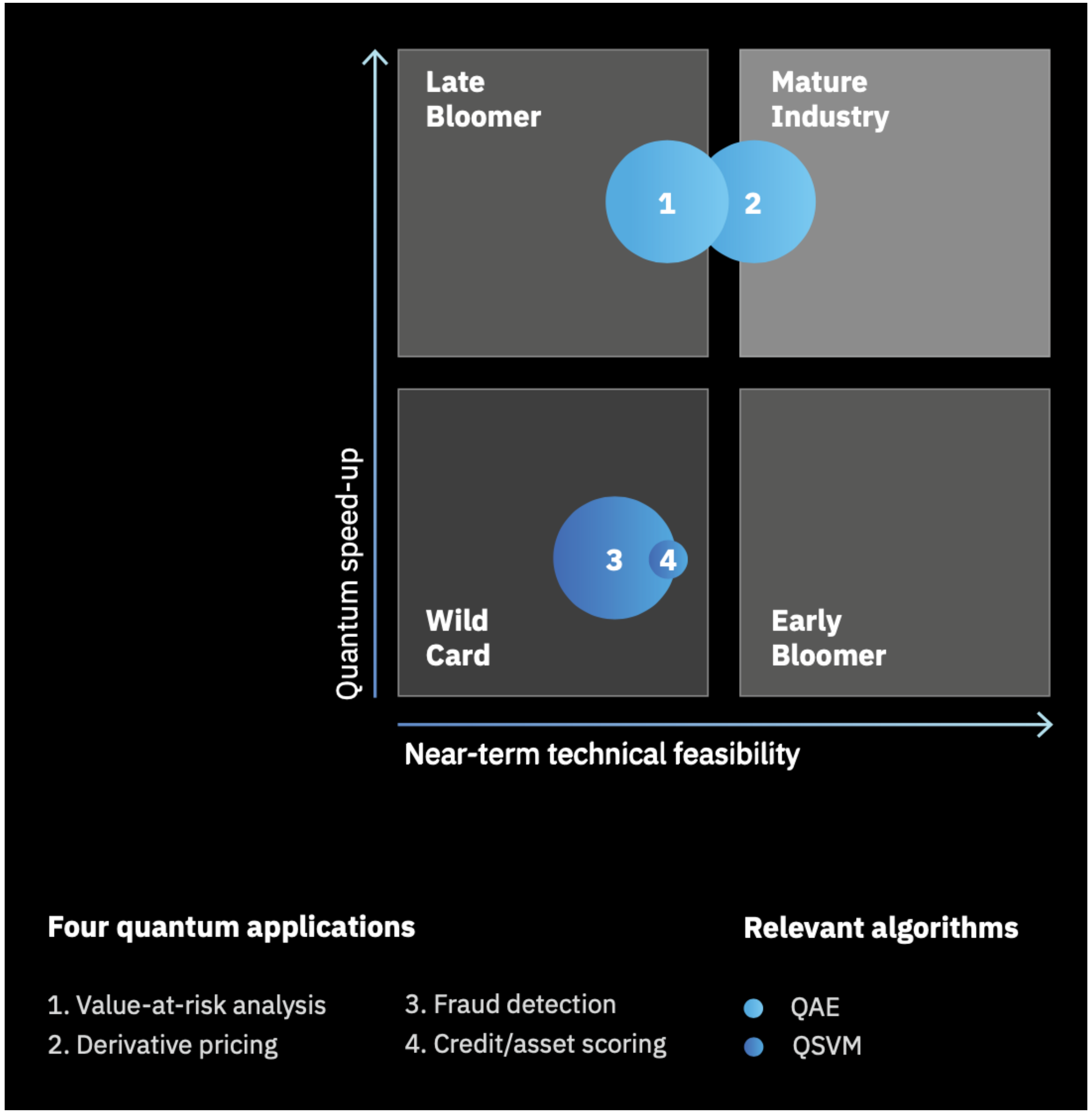


Prioritising Framework

Quantum speed-up: Theoretical capacity to deliver technological advantage over classical computing solutions (Y-axis)

Near-term technical feasibility: Operational readiness (X-axis)

Relative potential business impact by use case: Ability to drive unique business value for a specific enterprise (bubble size)



Selecting the right Quantum Project for your organisation

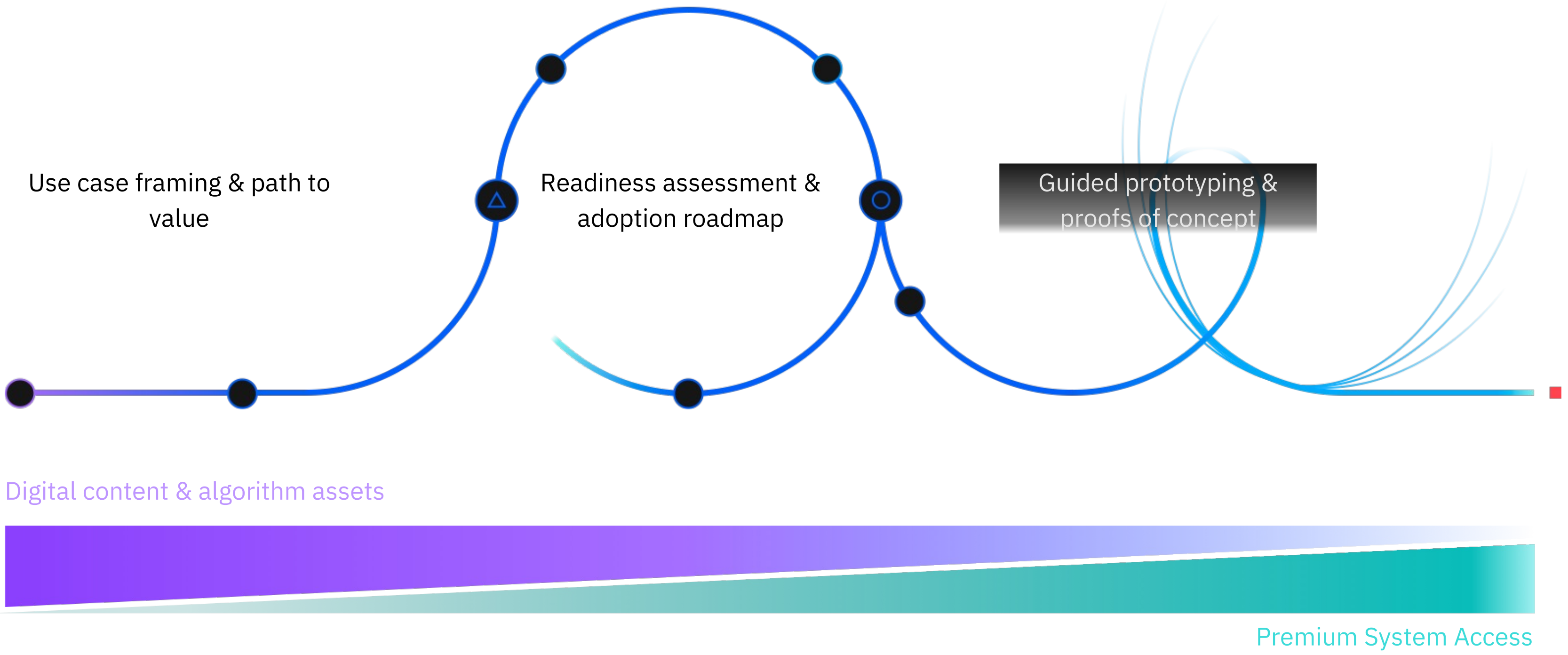
- What Technical Skills do you have in your organisation
- What applications are important for your organisation
- Where will your work fit in the prioritization matrix – will it get you business value?

Our offering to prepare your organization for quantum advantage…

Business readiness:
Define your company's compelling case for quantum. Set priorities to capture new opportunities and minimize risk of competitive threats. Develop early proofs of concept with experts in industry quantum computing.

Technical readiness:
Build quantum fluency across your organization and engage technical teams in learning experiences with hands-on applications of quantum algorithms through guided prototyping.

Premium access:
Direct access to premium quantum services and support for the world's most advanced fleet of quantum systems.



Volume 20, Issue 22
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Journal of Chemical Theory and Computation

Publishing reports on new theories, methods, and important applications in quantum electronic structure, molecular dynamics, and statistical mechanics.

2 Year Impact Factor 2023: 5.7 | Citations 2023: 49,731 | CiteScore 2023: 9.9

BIOMOLECULAR SYSTEMS | November 6, 2024

Protein Structure Prediction with High Degrees of Freedom in a Gate-Based Quantum Computer

Jaya Vasavi Pamidimukkala, Soham Bopardikar, Avinash Dakshinamoorthy, Ashwini Kannan, Kalyan Dasgupta*, and Sanjib Senapati*

Thank you