ACS Edition



Introduction Quantum devices and machines Fundamental principles Developing quantum solutions Quantum computing in action Benefits, challenges and opportunities Summary, reflections and questions

Quantum computing is modern magic Quantum machine learning turns data into magic

IBM quantum computer

Business Applications of Quantum Computing: Opportunities and Challenges for Software Developers ACS Edition

Honorary Assoc. Prof. Jacob L. Cybulski School of IT, SEBE, Deakin University

What is Quantum Computing?

Quantum mechanics

is the area of science dealing with the behaviour of matter and light on the atomic and subatomic scale (Britannica.com, 2020)

It is the foundation of all quantum physics including quantum chemistry, quantum field theory, quantum technology, and quantum information science (Wikipedia.org, 2021)

Quantum computing and *Quantum information science*

suit complex problems with little data

suit complex problems

Quantum

Technology

with lots of data

are the study of the information processing tasks that can be accomplished using quantum mechanical systems (Nielsen and Chuang, 2010)

Quantum machine learning, Quantum optimisation, Quantum cryptography, Quantum communication are IT-related quantum technology sub-fields

Quantum engineering (building quantum devices) is the quantum area attracting the majority of global effort

Qubit is the fundamental concept in quantum technology It is a unit of quantum information

It is also a device able to manipulate a single unit of such information



Australian quantum landscape: A\$1b Critical Technologies Fund

(2022)

- Critical Technologies Fund is part of the \$15b initiative National Reconstruction Fund which aims to strengthen Australian industry
- A\$1b will be Invested in 63 technologies, including *Quantum Technology*
 - Quantum cryptography
 - Quantum communication
 - Quantum computing and
 - Quantum sensors

- Other technology areas, which are known to have benefited from quantum tech, are also funded under the scheme, e.g.
 - Advanced materials and manufacturing
 - Artificial intelligence
 - Biotechnology
 - Energy and environment
 - Sensing, timing and navigation
 - Transportation, robotics and space

Australian Quantum Alliance

- Several members in the advocacy group of companies known as Tech Council of Australia formed *Australian Quantum Alliance*
 - The group includes local and global leaders in quantum technology

- The alliance aims to:
 - Promote quantum technology to the industry

(2022)

- Provide advice to government on the relevant policy issues
- Build partnerships with key international and local stakeholders



Australian quantum activity



Ouantum hardware

software

- sensors
- applications + education

- The University of Melbourne
- Monash University
- Swinburne University
- Victoria University

Australian **Quantum Industry**

Archer

Rigetti Computing (US)

Olivier Ezratty. Understanding Ouantum Technologies. p 732, 2021. http://arxiv.org/abs/2111.15352.



Main research players

fundamental research and quantum hardware

- University of Sydney with Microsoft
- UNSW with Silicon Quantum Computing
- University of Melbourne with IBM Quantum

Outside Victoria

ANU (Department of Ouantum Science and Technology) UTS (Centre for Quantum Software and Information) Macquarie Uni Sydney (Centre for Quantum Engineering) Griffith Uni (Centre for Quantum Dynamics) Uni of Western Australia (Centre for Ouant Info. Sim and Algorithms) Uni of Queensland (Centre for Quantum Optics and Quantum Information)

Also we must not forget: Sydney Quantum Academy (Sydney, NSW) Quantum Terminal at Central Station (Sydney, NSW)

Victorian Quantum **Technology Network**

- Deakin University
- **Federation University**
- La Trobe University

Quantum sectors

Consultancy

- **RMIT University**

Global Quantum "Thought" Giants (2021-2022)

Universal / Gate-Based Machines

- IBM (Superconducting / Cooper pair)
- Google (Superconducting)
- Rigetti (Superconducting)
- IonQ (Trapped ion)
- Honeywell (Trapped ion, with CQC)
- Microsoft (Hybrid+Topological)
- AQT Alpine Quantum Tech (Trapped ion)
- CEA Leti (Spin Silicon / Photonics)
- Quantum Brilliance (Carbon / Room Temp)
- Xanadu (Photonics / Room Temp)
- Baidu (Superconducting)

Quantum Annealing Machines

D-Wave (Q Annealing+...Gate based)

Simulators / Quantum Inspired

- Atos (GPU, 41 qubits)
- Alibaba (Cloud QPD)
- Fujitsu (Digital Annealing)

Software-PaaS / QC

- ETH Zurich ProjectQ
- CQC (Cambridge) t|ket>
- Classiq Q synthesis engi
- IBM Quantum Qiskit
- Google Quantum AI Cirq
- Microsoft Azure Quantum QD Kit/Q#

Ragot, Sébastien, and Michel Kurek.

"Ouantum Technologies: Patent Applications vs. Scientific

Publications across the World." LinkedIn, November 4, 2021. https://www.linkedin.com/pulse/quantumtechnologies-patent-applications-vs-scientific-ragot/.

AWS Braket - Amazon Braket SDK

Software-PaaS / QML

- IBM Quantum / Qiskit Qiskit ML
- Tensorflow TFQ (+Cirq)
- Xanadu PennyLane (+SF)
- Atos QLM

Applications / Users

- NASA, BASF, Boeing, VW, ...
- Accenture (Business)
- Zapata (Business)
- 1QBit (Medical / Finance)

c.38%

Breakdown of patent applications (2010-2021)

Europe Japan Korea Canada Australia

China

India

Providers

- Quantinuum
- lonQ
- QCI
- Rigetti
- Pasqal
- 1QBit
- Microsoft QIO
 Toshiba
- Rigetti [•] ^{10SI}
- OQC

Providers

lonO

- Xanadu
- Q-Wave OuEra (soon)

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Global Government Initiatives



- Australia (US\$94M+%A\$1b)
- Canada (US\$66M+US\$360M)
- China (US\$10B)
- EU (US\$1.1B)
- Finland (US\$25M)
- France (US\$1.8B)
- Germany (US\$3.1B)
- India (US\$1B)
- Israel (US\$360M)

- Japan (US\$470M)
- Netherlands (US\$740M)
- New Zealand (US\$25.5M)
- Russia (US\$663M)
- Singapore (US\$109M+US\$74.8M)
- South Korea (US\$37M)
- Sweden (US\$115M)
- UK (US\$1B)
- USA (US\$1.275B)

Quantum tech: past, present and future Fears, expectations and myths?



Past and Present (last 5-10 years)

- Q machines are still part of the NISQ generation (small and noisy)
- Q machines require very large and complex infrastructure to run
- They are no longer just a theory!
- Q development requires specialist skills and knowledge (e.g. Maths)
- Q algorithms are being developed
- Q applications are mostly proofs of concept, not of industry strengths
- Q advantage can be demonstrated in specific areas where Q approaches are an improvement over classical ones
- Q supremacy still cannot be proven

Very Near Future (5-10 years)

- Q breakthrough-tech will be rapidly developed leading to new Q solutions
- Q machines will feature over 1000 qubits
- Q tech will deal with noise and decoherence to allow useful computation
- Q cloud services will become widely available at low cost on pay-for-use basis
- Q and classical tech will become integrable and flexibly scalable for business
- Q computers for SMEs and individuals will be small and operate in room temperature
- Q long-term memory and Q networks will be developed to support large-scale Q systems
- Q software will become easy to use

Quantum Devices and Machines

Quantum technologies that are currently being explored include:

- Quantum sensing systems (incl. measuring instruments)
- Quantum information systems (incl. cryptography)
- Quantum communication (incl. networks)
- Quantum computers (focus on NISQ* machines)
- Quantum inspired systems (incl. new classical algorithm and special-purpose hardware)

Quantum computers may operate using vastly different approaches:

- Quantum circuit/gate computers (incl. quantum supremacy)
- Quantum simulators (incl. HPC quantum accelerators)
- Quantum annealing computers (incl. quantum adiabatic computation)
- Topological quantum computers (incl. anyons, Majoranas and braids)
- Universal quantum computers (incl. Quantum Turing Machines)

(2021-2022)

Quantum Machines

Achieved quantum supremacy performing Gaussian Boson Sampling (GBS)

University of Science and Technology of China in Hefei (*Jiuzhang 2* - Photonic)



Baidu Qianshi (Superconducting)



Google (Superconducting)

Rigetti (Superconducting)





Atos Quantum Learning Machine





IBM (Superconducting)

Xanadu (Photonic)





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Trends, progress and timelines IBM Quantum Development Roadmap



Prerequisite Knowledge to enter QC / QML / QO work

Quantum Computing

- A subset of Quantum Mechanics
 - Complex numbers
 - Linear algebra
 - Probability theory
 - Statistics
- Programming (mainstream)
 - Python (with APIs)
 - OpenQASM
 - ✓ Q#
 - Silq
 - **ب**

Quantum Hardware

- Configuration
- Calibration
- Error mitigation

Quantum Machine Learning / Quantum Optimisation

- Quantum computing
 - Quantum algorithm design
- Data science / Maths and algorithms
 - Calculus incl. differential equations, PDE
 - Optimisation techniques incl. gradient descent, quadratic programming
 - Machine learning incl. algorithms, models, training, validation, differential programming, and more...

Qubits In a simplified way!

Qubit is a device representing a unit of quantum information, which is often "implemented" as a single elementary particle, e.g. electron or photon

Qubit represents a state of such a particle, e.g. an electron spin (<u>up</u> or <u>down</u>) or photon's linear polarisation (<u>horizontal</u> or <u>vertical</u>)

Qubits are in a state of *superposition* of some *basis states*, so the electron spin is not just \underline{up} or <u>down</u> but a combination of these states, e.g.

$$\frac{\sqrt{3}}{2} \times \underline{up} + \frac{1}{2} \times \underline{down}$$

When we *measure* the qubit, its state collapses probabilistically into one of the basis states |0> or |1>, measured as simple values, e.g.

- "0" / "1" for <u>up</u> or <u>down</u> for electrons, and
- "0" / "1" for <u>horizontal</u> or <u>vertical</u> for photons.

What does it all mean?

- What is a qubit state?
- What are basis states?
- What is superposition?

It seems, Nature works in a purely mathematical way!

Mathematically a qubit state can be represented as a vector (a point) in space of all possible qubit states. The state space has its own coordinate system, which is defined by the basis vectors, which are orthogonal unit vectors (length=1), for example in 2D these could be vectors (1, 0) and (0, 1), which in quantum physics are denoted as |0> and |1>.



As we can see, any vector (a, b) is a (linear) combination of the basis vectors (1, 0) and (0, 1) – we call this *superposition*.

Qubits In a complex way!





Qubit visualisation

As the qubit state is described by two complex numbers, we will need to visualise four dimensions

$$(\alpha_1, \alpha_2, \beta_1, \beta_2)$$

However, with a clever "projection" trick we can depict the qubit state in 3D, e.g. as a *Bloch sphere*.

Bloch sphere represents a single qubit state in *x*, *y*, *z* Cartesian coordinates, as well as by θ and ϕ angles in polar coordinates (*amplitude* and *phase*)

A typical quantum operation (called "gates") is the *rotation of qubit state* around x, y or z axis, which is moving the state vector on the surface of the Bloch sphere.

Note 1: In this visualisation the angle θ between orthogonal states $|0\rangle$ and $|1\rangle$ is shown as 180° rather than the actual value 90° (this impacts some calculations).

Note 2: Phase ϕ has no impact on the outcome of a qubit measurement! (self-evident, see the figure)

Note 3: When qubit state is placed in the middle of the basis states (using the Hadamard gate "H"), then measurements "0" and "1" are returned with 50% probabilities.

• *Qubit state* ψ is a vector in *superposition* of two basis vectors:

Dirac or bra-ket notation

Computational basis
$$ightarrow \left\{ \left| 0 \right\rangle
ight.$$
 , $\left| 1 \right\rangle$

 $\left|\psi
ight
angle=lpha\left|0
ight
angle+eta\left|1
ight
angle$ and $\left|lpha
ight|^{2}+\left|eta
ight|^{2}=1$

where α and β are complex numbers, referred to as *probability amplitudes*.

• When measured, the qubit state collapses (is "projected") onto its basis states resulting in an observation of value of either "0" or "1".

Probability amplitudes α and β can be used to determine the probability of measuring this outcome:

$$p(0)=\left|lpha
ight|^{2}$$
 and $p(1)=\left|eta
ight|^{2}$

Multiple qubits + Entanglement

What happens when we have two independent qubits q_1, q_2 in states ψ_1 and ψ_2 ?



The state of this composite quantum system is a superposition of:

 $\{ |00\rangle\,,\,\,|01\rangle\,,\,\,|10\rangle\,,\,\,|11\rangle\}\,$ computational basis.

The composite system

Note that the dimension of the composite state space is exponential of the number of qubits, i.e. for 2 qubits we have 2² states, for 3 gubits we have 2³ states, etc.

What happens when two dependent qubits q₁, q₂ are placed in the following initial states:



We measure this quantum system, and:

- when qubit q_1 is measured, its value will be 0 or 1 with equal probability, then...
- when $q_1 = 0$, q_2 state will stay as 0, when $q_1=1$, q_2 state will flip to 1.

Measurement of both gubits is always the same the gubits are entangled.

15/26 $|\rangle\rangle\rangle$, $|11\rangle$ } $\{ |00 \rangle,$

Quantum programs Quantum circuits

- Quantum programs, e.g. in Python, aim to construct and execute a quantum circuit
- Quantum circuit is the fundamental model of quantum computation
- A circuit identifies a number of quantum qubits and their initialisation
- A circuit also defines a sequence of quantum gates responsible for performing operations on these qubits
- There are different types of gates, e.g. single qubit gates (e.g. qubit rotations), two-qubit gates (e.g. conditional ops), and multi-qubit gates which can all be defined in terms of single and two-qubit gates
- The circuit also defines measurements, which allow observing qubit states (as a side-effect qubit states collapse and qubits may be destroyed in some systems)

Quantum circuits and gates may have very different forms and types depending on hardware

On IBM superconducting quantum machines, circuits are prepared and loaded into inter-connected quantum hardware, supporting only specific gates, and executed



On Xanadu photonic quantum machines, circuits are "ephemeral" where qubit states are made with light and circuits are continuously executed in the process, they also feature gates such as "beam splitters" (BS) and "phase shifters" (R) manipulating light beams



Building a quantum solution A typical setup of a circuit





In the process of quantum circuit design, we usually perform four tasks (opt. interspersed and repeated), i.e.

- 1) Initialisation of quantum registers, commonly to |0>
- 2) Preparation of quantum information, which involves setting each qubit to a specific state based on input data
- 3) Processing of quantum information, which applies inter-related gates to these qubits
- 4) Measurement of qubits to obtain classical information about their state

A circuit can then be executed, but note:

Input data is hard-coded into the circuit! Different input requires a new circuit

Each execution produces a single random result! A circuit must be executed repeatedly, measurements collected and their distribution analysed

When the circuit is too deep, its qubits and gates may decohere due to noise, leading to errors! Presence of noise requires detailed analysis of results, error mitigation, or circuit redesign

Example Entanglement on NISQ machines

- When two qubits are independent, their measurements are also independent
- Take the following two independent qubits, their measures of "0" or "1" are with equal probability:



The state of two qubits can be described as a superposition of their computational bases |00>, |01>, |10> and |11>

On NISQ machines circuits decohere during execution, and errors are produced. When we execute circuits repeatedly we need to carefully interpret distribution of results for both the expected results and for errors.

- However, when the qubits are *entangled*, i.e. their measurements are correlated.
- Take as an example the following qubits entangled in a *Bell state*:



When the circuit is executed repeatedly, all possible outcomes are produced with **equal probability**.

Distribution of results obtained from 1024 runs reflects a truly random nature of qubit measurement



The circuits are now executed on a NISQ machine 1024 times

 Their measurements should **always** be the same, though the measured values can be random.



Quantum Machine Learning Variational (parametrised) circuits

Note that any circuit before execution is normally transpiled, i.e. translated into the form suitable for execution on the specific quantum computer

Optimisation Algorithm



which can be optimised using an ML algorithm.

The optimisation is iterative and works as follows... At each optimisation step a template is instantiated by filling in *input parameters* with training data, and *process parameters* with values provided by the optimiser to create an updated quantum circuit. The circuit is executed and its outputs measured. The measured output values are interpreted and compared against the expected values using a cost function, and the optimiser determines the new set of values for the process parameters.

OS quantum algorithms The ever growing quantum tool-kit!

QC

pure quantum

- Bernstein-Vazirani Algorithm
- Grover's Algorithm
- Shor's Algorithm
- Quantum Fourier Transform
- Quantum Teleportation
- Quantum Key Distribution
- Quantum Image Processing
- HHL Alg. (lin eqs solver) ...

Protocols / Patterns

- Random Number Generation
- Quantum Phase Estimation
- Quantum Counting
- Quantum RAM (qRAM) ...

Variational

- Variational Quantum Eigensolver (VQE)
- Variational Quantum Classifier (VQC)
- Variational Quantum Linear Solver (VQLS)
- Quantum Kernels and Feature Maps ...

Quantum Machine Learning

- Quantum k-Means and k-NN
- Quantum Approximate Optimization Alg. (QAOA)
- Quantum SVM (QSVM)
- Quantum Neural Nets (QNN) and ConvNets (QCNN)
- Quantum Generative-Adversarial Nets (QGAN)
- Quantum Boltzmann Machines (QBM) and VQBM
- Quantum Reinforcement Learning (QRL)
- Quantum Annealing ...

Vendor provided application development tools

- Quantum technology vendors provide many standard packages for solving typical business problems
- For example, IBM Qiskit offers four classes of quantum applications, for solving problems in areas such as:
 - natural science, such as calculation of molecular states or protein folding;
 - finance, such as portfolio optimisation, pricing of financial options or credit risk assessment;
 - optimisation, such as in vehicle routing or energy distribution using several quantum-enhanced optimisation techniques;
 - machine learning, featuring many general purpose algorithms, such as neural networks or kernel methods.

- Quantum applications can demonstrate their advantage over classical solutions by relying on the following features of quantum systems:
 - True randomness of quantum results (via quantum measurement)
 - Pursuing many decision paths concurrently (via quantum superposition)
 - Controlling parallel choices with constraints (via quantum entanglement)
- An example where all three principles are applied – financial option price prediction



Published quantum applications

Often proofs of concept awaiting large and robust quantum computers

Selected Areas

- Cyber security
- Financial services
- Materials / manufacturing
- Transport / logistics
- Aerospace / automotive
- Energy / resources
- Medical / healthcare
- Chemistry / pharmaceutical
- Bio-tech / genetics / omics
- Sensors / measurements
- and more...

Illustrative Examples

Breaking classical encryption, post-quantum methods Portfolio optimisation, fraud indicators, credit scoring Structural analysis, efficient batteries, costs and risks Supply chain / inventory / distribution optimisation Efficient fuels, effective assembly, route planning Energy distribution, planning and optimisation Results of therapies, prediction of adverse effects Chemicals with new properties, drugs, personal medicine Protein folding, study of genetic diseases Precise instruments, timing, navigation, imaging

Major players in quantum application

- Defence Systems Cryptography, planning, control, sensing, etc.
- NASA (QuAIL) Mission control, space vehicle / rover design and coordination, air traffic management, planning and scheduling, fault diagnosis, etc. https://www.sciencedirect.com/science/article/pii/S0167819116301326
- Accenture Financial, logistics, communications and security services https://www.accenture.com/au-en/services/technology/quantum-computing-services
- BASF Quantum chemical computations: new catalysts and polymers https://www.qutac.de/basf-how-quantum-computing-can-help-develop-chemical-catalysts/?lang=en
- Ford / VW / BMW Traffic, batteries, financials, materials, production opt https://spectrum.ieee.org/ford-signs-up-to-use-nasas-quantum-computers https://www.volkswagenag.com/en/news/stories/2021/08/volkswagen-takes-quantum-computing-from-the-lab-to-the-factory.html https://www.zdnet.com/article/bmw-explores-quantum-computing-to-boost-supply-chain-efficiencies/
- Boeing / Airbus Manufacturing, materials, logistics, aerospace, flight dynamics https://www.ibm.com/blogs/research/2020/09/quantum-industry/
- Goldman Sach / JPMorgan Financial: derivatives, simulations, pricing, etc. https://www.efinancialcareers.com.au/news/2020/12/quantum-computing-at-goldman-sachs-and-jpmorgan
- Boehringer Ingelheim Medical molecular dynamics
 https://www.boehringer-ingelheim.com/press-release/partnering-google-quantum-computing

Quantum technology benefits & challenges

Benefits of quantum tech

- Seamless integration of algorithms with maths and physical phenomena
- Best at hybrid quant/classical solutions
- Solve complex/seemingly impossible problems efficiently in selected domains
- Effective sampling devices and truly random number generators
- Handling of massive parallelism with effective constraint satisfaction
- Cloud-based QC lowered access costs
- Plethora of free QC learning resources, courses, study groups and hackathons
- Increased awareness amongst business
- Huge interest of serious developers

Quantum tech challenges

- Difficult to conceptualise, design, develop, execute and understand results
- Quantum advantage can only be demonstrated in niche application areas
- Quantum supremacy cannot be proven
- Discrepancy between classical machine learning and quantum computing
- Quantum computing requires highly specialised skills (maths and physics)
- Shortage of knowledge, skills and expertise in quantum development
- No clear path of transitioning quantum proofs of concept to business applications
- Shortage of high-level development tools
- No SDK/SDE for post-NISQ machines with "high quality millions of qubits"
- No "software engineering" methods applicable to quantum development 2

Opportunities for R&D

Research

- Study post-NISQ quantum circuit development (1000s of qubits)
- Develop new QC user interfaces for nonscientists and business users
- Develop new creative and technical areas within QC development, e.g. quantum arts and music
- Translate / re-imagine / replace existing classical algorithms into quantum enhanced algorithms
- Establish large cross-institutional research groupings and joint centres
- Seek industry partners with problems suitable for quantum computing
- Establish research QC vendor relationships and funding opportunities

Development

- Develop programs to educate future QC developers, e.g. designers, programmers, testers, GUI developers, etc.
- Explore established QC application domains, e.g. chemistry, finance, logistics, etc.
- Create novel areas of QC application, e.g. computer vision, epigenetics, space, economics, fluid mechanics, etc.
- Develop high-level cross-platform quantum development environments (CASE / VLSI?)
- Establish cross-platform quantum reuse repositories and circuit generators
- Develop QC development methodologies
- Create QC software development interest groups / professional bodies
- Attract local QC venture capital

Bird-view of quantum computing... Summary, reflections and questions

Opportunities for Quantum R&D Quantum solutions for business

Free quantum learning resources New quantum tech products and services



New ways of solving "impossible" problems Variety of quantum tools and methods for developers

Australian Governments quantum initiatives Quantum enabled discoveries in science

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