Quantum Computing & Simulation Hub

Quantum Simulation

An overview of quantum simulation and its applications

Summer 2022



Publication Information

This is a publication from the **Quantum Computing & Simulation Hub,** an EPSRC funded collaboration of seventeen universities, bringing together academia and industry as part of the **UK National Quantum Technologies Programme.**

This report was authored by: Christopher Noble, Adi Sheward-Himpson, Evert Geurtsen, Rupesh Srivastava and Celia Yeung.

1.1.J.J.S.L.

Acknowledgements

The authors would like to thank, in no particular order, the following individuals for their invaluable support and advice throughout the creation of this report: Andrew Daley, Anthony Laing, Stefan Kuhr and Ulrich Schneider.





Introduction

Quantum simulation is an often overlooked part of the Quantum Information Technology (QIT) revolution that is currently happening around the world. QIT promises new approaches to computing, inherently secure communications and the ability to solve intractable computational problems. However, perhaps one of the most essential offerings will be a better ability to understand nature and its fundamentals.

Existing digital computers make valiant attempts to mimic the complex processes we find in nature, but despite the ever increasing and cheaper volumes of processing power, few can match the complexity of quantum physics. For many of the most fundamental problems – often the most valuable in chemistry and physics – classical computing proves to be inadequate. Quantum computers are expected to perform better in these areas, but the best modelling of quantum dynamics could be provided by a quantum system that we can manipulate. This is known as a quantum simulator.

Developing these tools faces tough technological challenges, but good progress is being made towards practical applications in industry and science. Quantum simulators offer unique strengths and should be considered as viable near-term solutions for high-value applications in fields such as logistics, materials discovery and chemistry. This report provides an accessible overview of quantum simulators, their technology and their likely applications. <image>

Professor Dominic O'Brien Director, Quantum Computing and Simulation Hub

Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.

Richard Feynman

What are quantum technologies?

The behaviour of nature at the atomic and subatomic scales has intrigued and divided scientists, writers and philosophers over many decades. This branch of physics, called 'quantum mechanics', has given us incredible insights in how nature operates beyond our everyday experience, and introduced new terms like *superposition, entanglement, interference, tunnelling and teleportation.*

Now we are at the stage where we can harness these unique properties of the quantum world and, coupled with quantum information science, engineer entirely new technologies across imaging, sensing, timing, communication, computation and simulation.

Imagine being able to discover new materials and medicines, optimise logistics, and enhance online security – these are just some of the applications being pursued by researchers and businesses across the world.

Why simulation matters

Simulation is the representation of some physical or natural system by another, in order to advance understanding, explore theories and predict outcomes. Simulation is not a new concept – planetary motion, for instance, has long been of interest and various physical models have been constructed throughout the ages. [1]

Electronics and digital computing have played an important role in advancing simulation techniques. The first electronic analogue simulator was proposed and developed in 1938 by George A. Philbrick, an 'Automatic Control Analyzer' which saw considerable use as a training tool. [2] Analogue computers have seen use in subsequent decades in applications such as modelling control systems (e.g. flight simulators). [3]



The first modern orrery can be traced to English clockmakers George Graham and Thomas Tompion in 1704.

Image © History of Science Museum, University of Oxford, inventory no. 45104

66

In just a few minutes of demonstration, it could impart considerable knowledge of process dynamics, controller tuning, and the effects of load and control-point upsets.

77

George A. Philbrick [2]

Nowadays, common applications for simulation include: designing buildings and other complex structures, studying chemical processes, analysing vehicle aerodynamics, and modelling geological activity, the behaviour of crowds and even the spread of disease. [4] [5]

Simulation vs Emulation

The terms *simulation* and *emulation* are often used interchangeably to suggest the representation of one system on another but in the context of this report, they are different entities.

A *quantum simulator* is a physical quantum system used to model another quantum system (or a problem that can be mapped to it, such as optimising traffic routing for example).

An *emulator* is used to represent hardware. For example, quantum computers can be emulated in software (up to a point) while the hardware is being developed. The open source software QuEST is one such emulator, used by researchers to run quantum algorithms on a variety of problems. [6]



A RAT 700 analogue computer (left) simulating a car suspension system in the scope (right)

Source: Hobby - Das Magazin der Technik, issue 6, 1965

Simulation and analysis market history and forecast

With digital computers becoming more powerful and cheaper, there is an increasing demand for engineering simulation and tools, with the global market for the simulation and analysis industry forecast to exceed \$10 billion by 2024. [7] Analogue quantum simulation will be a very interesting addition to this growing field.

CIMdata Publishes Simulation and Analysis Market Report. [7]



Source: www.cimdata.com

Global simulation software market share, by end-use, 2020 (%)



Source: www.grandviewresearch.com

adod why do do

Simulation



Simulators can help us to understand real-world behaviours that are too big, too small, too expensive, too far away or too dangerous to study directly. As this report shows, they are emerging as a key tool in areas that cannot be tackled using existing technologies, including natural quantum systems (e.g. in chemistry or particle physics) and similarly complex phenomena.

The advent of quantum simulators brings new tools for studying systems and quantum systems in particular, offering capabilities beyond the reach of classical computers. [8]

Image Credit: Ulrich Schneider

Digital vs Analogue

When we speak of an analog quantum simulator we mean a system with many qubits* whose dynamics resembles the dynamics of a model system we are trying to study and understand. In contrast, a digital quantum simulator is a gate-based universal quantum computer which can be used to simulate any physical system of interest when suitably programmed, and can also be used for other purposes.

Analog quantum simulation has been a very vibrant area of research for the past 20 years while digital quantum simulation with general purpose circuitbased quantum computers is just now getting started.



* A qubit is the most basic unit of information in QIT.

PAGE

Building analogue quantum simulators



Image Credits: (Top) KK Clark / Blogspot • (Bottom) Memetician / Livejournal

man

NISQ: Current digital quantum devices are error-prone, and typically limited in size to tens of qubits. We refer to the era as noisy intermediate-scale quantum, or NISQ.

A System View

Various technologies may be used to build quantum simulators. Each approach requires a multidisciplinary effort to integrate hardware and software, possibly with cloud services potentially providing remote access to a range of global users.

Right: High-level system view of the components

J.J.J.S.S.A.

required for useful quantum simulators



There are other important considerations in the development of quantum simulators:



Quantum Simulator Technologies

Quantum simulators share many of the same base technologies as quantum computers. These include ultracold (aka neutral) atoms, trapped ions, superconducting, and photonic systems. A comparison of these is shown below. Other candidate technologies include quantum dots and colour-centres in diamond, which are still relatively early in their development phase and are not included here.



Trapped lons

Charged particles trapped in electromagnetic fields.

Trapped ions (based on a chain of ionised atoms trapped in rotating electromagnetic fields) are heavily developed for digital quantum computing. Spins can be encoded on the internal electronic states, and controlled with laser light. Spin models with long-range interactions can be implemented directly, mediated by the collective motional modes of the system of trapped ions. In the last few years they have been used to study out of equilibrium dynamics, and to implement variational quantum eigensolver routines. The challenge is to scale this beyond ca. 50 ions in a single trap, either by working with 2D arrays of ions, or by generating electronic or photonic interconnects between traps **Examples: IonQ, Quantinuum, Universal Quantum**



Superconducting Circuits

Superconducting electronic circuits.

Superconducting qubits are presently one of the most developed architectures for quantum computing, based on well-developed microwave technologies and micro- or nano-electronic circuits that are cooled to milliKelvin temperatures. For quantum simulation, these platforms can also be used to explore the dynamics in a variety of spin and bosonic models. Existing systems with around 100 qubits have been used to study advanced models of condensed matter physics, demonstrating the applications of these hardware platforms for fundamental science. The next stage of development will involve scaling to larger numbers of qubits while improving the local calibration of qubits. **Examples: Google, IBM, Rigetti**



Photonics

Uses photons as information carriers.

Programmable photonic circuits are well suited to simulating so-called "bosonic" systems, such as vibrations in molecules. Quantum states of light such as ensembles of photons or squeezed states can be injected into miniaturised and interferometrically stable chips, made from silicon or other materials. Chip-scale reconfigurable systems with up to 18 photons have been demonstrated, within the limit of what can be simulated with classical computers. Larger scale systems of >100 photons with small levels of programmability have challenged the capabilities of supercomputers to simulate experiments at this scale. The next stage of development will include the introduction of programmability and error mitigation.

Examples: Duality Quantum Photonics, Orca Computing, Photonic Inc, Xanadu



Ultracold Atoms

Programmable lattices of cold atoms.

Ultracold atoms trapped in laser light can be used to build lattice models usually used to describe electrons moving in a solid crystal, with atoms moving in crystals of laser light (an "optical lattice"). Neutral atoms have the unique benefit that they can directly implement models for fermions (like electrons), and this has been applied to study problems in condensed matter physics in the past few years. The state of the art involves over 1000 atoms in a 2D lattice (or ca. 250 trapped in optical tweezers, implementing spin models through Rydberg excitations). Individual addressing has been realised in quantum gas microscopes, and the next steps will involve improvement of local calibration.

Examples: Atom Computing, Pasqual, QuEra

Image Credits: (Top Left) David Nadlinger • (Top Right) Jay M. Gambetta, Jerry M. Chow, and Matthias Steffen, under CC BY 4.0

Illustration of an optical lattice-based quantum simulator

An overview of a cold atom-based quantum simulator is shown below.



Image Credit: CHIP magazine / Immanuel Bloch • https://tinyurl.com/chip-magazine

PAGE 08

The practical uses: applications

The range of applications for quantum simulators covers fundamental areas from science and metrology through to industrial processes. Examples in various categories are shown.





Cold Atoms in Space – CAL and BECCAL.

In 2018, NASA launched "CAL", the Cold Atom Lab, to the International Space Station (ISS). CAL's purpose is to study quantum phenomena and future quantum sensors based on laser-cooled atoms of rubidium and potassium. [11]

In contrast to earth-based laboratories, the microgravity environment of the ISS enables longer observation times (over 10 seconds) and even cooler temperatures (< 100 pK is possible) making a wider range of experiments possible. [12]

The successor to CAL, called "BECCAL" – Bose-Einstein Condensates and Cold Atom Laboratory (Below), is being planned in collaboration with DLR, the German Aerospace Centre, to be launched in 2025. [13]



Source: https://arxiv.org/pdf/1912.04849

Sugar why do a



Nature cover from June 2020: Bose-Einstein Condensates created in orbit for the first time.

Read more here: https://coldatomlab.jpl.nasa.gov/news/nature-cover/

Quantum simulator specialists

The majority of expertise in quantum simulation lies in university research groups world-wide, funded by government or through international collaboration, such as the EU Quantum Flagship*. This field is nascent but growing, and continued international cooperation is essential to accelerate innovation.



The shoots of progress can be seen in the emergence of commercial entrants with a small user community. Some organisations have been given early-access to prototype devices, while others are actively exploring applications on more mature platforms that could give them a business advantage across a variety of industry sectors.

A research group, businesses and a large-scale project are highlighted on the next page to illustrate activities in the field.

* One of the largest and most ambitious research initiatives of the European Union, with a budget of at least €1 billion and a duration of 10 years. [14]



SPOTLIGHT

From 51 to 256 atoms in 3 years



rle mit edu

Atoms announced a 51 qubit neutral atom simulator to model interactions between certain atoms. [15]

In 2017 a team led by the MIT-Harvard Center for Ultracold

Three years later this team demonstrated a substantial update – a programmable 256 atom simulator to explore quantum phases of matter. [16]

PASQuanS – A €10m, multinational Flagship project

Pasqal – 1000 qubits in 2023?



pasquans.eu

PASQuanS is an EU Quantum Flagship project, which ran from 1st October 2018 to 31st March 2022. 14 partners across 5 countries (Austria, France, Germany, Italy and the UK) collaborated to improve control methods and develop fully programmable simulators, with an ambition to scale from 20 to more than 1000 atoms or ions. [17]

QuEra – Cloud access to a programmable simulator

bed and a de



quera.com

QuEra launched in 2019, with a team including leading researchers from the aforementioned 256 atom simulator. It exited stealth mode in 2021, with \$17 million in funding, and is providing customers access to its neutral atombased development machines with full-stack software. Its current analogue simulator has a specialized application in sampling probability distributions. [18]



PASQuanS is co-ordinated by Antoine Browaeys, who is also the co-founder and Chief Science Officer of Pasqal. Pasqal see quantum simulation as one of the most promising applications of their neutral atom technology [19] and, following their 2022 merger with Qu&Co, have announced a 1000 qubit quantum solution to be delivered in 2023. More information on Pasqal is available in the **Commercial Activities** Appendix.

UK Activity

Below is a map showing some of the research into quantum simulators happening in the UK, many with direct involvement with either the QCS Hub or the UK's National Quantum Technology Programme.

University of Strathclyde:

The University of Strathclyde has a large expertise in cold atom quantum simulation, with three quantum simulators with cold atoms in optical lattices, optical tweezer arrays, and a large theory programme on the design and application of quantum simulators.

University of Oxford:

Work across quantum simulation, including with cold atoms, trapped ions and superconducting systems, in both theory and experiment.

University of Bristol:

Specialises in photonics, investigating areas such as the simulation of molecular quantum dynamics, as well as theory of quantum simulators. Bristol runs the Quantum Engineering Technology Labs with over 100 academics, and has spun out Duality Quantum Photonics (see **Commercial Activities** appendix).

University of Edinburgh:

Research in the verification and application of quantum simulators.

Heriot-Watt University:

Work in the theory of quantum simulation with cold atoms and photons.

University of Nottingham:

Aiming to develop quantum simulators capable of providing insights into the physics of the very early universe and black holes. Part of the Quantum Simulator for Fundamental Physics (QSimFP) consortium.

University of Cambridge:

Significant experimental programme in quantum simulation using cold atoms in optical lattices and in continuum (QSimFP), as well as color centers in diamond. Related theory of condensed matter systems.

London:

Several London-based universities are actively conducting research into quantum simulation including QCS Hub partners Imperial College and UCL, with the latter also setting up the QLABS innovation centre. King's College are a QSimFP partner.

Research groups around the world

Below is a map showing some of the major national programmes and projects in quantum simulation around the world.



(QuEST) program.

Technologies.

4.1.J.S.S.C.

Oniversity of Queensiana
 Australian National University

Programming Quantum Simulators

The below examples illustrate the software which can be used when programming quantum simulators. There is not a hard boundary between quantum computing and simulation, and some of these will find application in both.

Low-level Control Software

Pulser from Pasqal

Pulser is an open-source software library (in Python) from Pasqal, a French startup developing neutral atom quantum technologies. Pulser facilitates the design and emulation of pulse sequences for neutral-atom quantum platforms, allowing for a range of tasks such as quantumcircuit programming and quantum simulation of many-body systems.



Above: Architecture of Pulser Source: https://arxiv.org/pdf/2104.15044

Quantum Operating System

Deltaflow.OS from Riverlane

Founded in 2016 in Cambridge, UK, quantum software company Riverlane is developing Deltaflow.OS, a quantum operating system for QIT devices.



Above: How Deltaflow.OS works. Source: Riverlane https://www.riverlane.com/products/

High-level Programming

Leap from D-Wave Systems

Launched in 2018, Leap is a quantum cloud service to access D-Wave's hybrid solver and QPUs (Quantum Processing Units) through an integrated development environment.





Above: Code sample Source: https://www.dwavesys.com/take-leap

How can my business leverage quantum simulation?

Quantum simulation requires a different approach to the usual 'wait until it's ready' adoption pattern. This is because it takes time to understand the technology, identify its potential value and impact, and build the necessary skills and partnerships to become quantum ready. The QCS Hub is available to assist businesses with this journey.





Sededade S. S. S.

New and emerging quantum simulators will support fundamental research in the laboratory, whilst commercial efforts are already producing early entrants into the market. Practical applications are imminent, with the capabilities of these devices applicable to fields outside of quantum – such as in logistics, whose total market value is estimated at circa \$10 trillion. [20]

Commercial Activities

There are a growing number of companies building quantum simulators for commercial exploitation. Some have been active for some time, others are very recent. A selection are shown below to illustrate activity in this field.



At a glance: Coldquanta is a spinout from the University of Colorado and develops quantum computers and quantum sensing technologies based on cold atoms. They offer a wide range of products and services, with a 100 qubit cloud-based quantum computer and high precision clock prototypes due to launch this year.









Contractor de ve

References and further reading

 J. Millburn, 'William Stukeley and the early history of the Orrery', *Annals of Science*, vol. 31, no. 6, 1974, pp. 511-513. DOI: 10.1080/00033797400200431.

[2] P. Holst, 'George A. Philbrick and Polyphemus – The First Electronic Training Simulator', *Annals of the History of Computing*, vol. 4, no. 2, 1982, pp. 153-154. DOI: 10.1109/MAHC.1982.10021.

 [3] A. Zazula et al., 'Flight Simulators – From Electromechanical Analogue Computers to Modern Laboratory of Flying', Advances in Science and Technology Research Journal, vol. 7, no. 17, 2013, pp. 51-52. DOI: 10.5604/20804075.1036998.

[4] P. Silva et al., 'Simulation – Concepts and Applications', in M. Lytras et al. (eds.), *Communications in Computer and Information Science*, vol. 112, Berlin, Heidelberg, Springer-Verlag, 2010, p. 429. ISBN 978-3-642-16323-4.

 [5] J. Sokolowski and C. Banks (eds.), Handbook of Real-World Applications in Modeling and Simulation, Hoboken, NJ, John Wiley & Sons, 2012. ISBN: 978-1-118-11777-4.

[6] QuEST, *QuEST – Quantum Exact Simulation Toolkit* [website], https://quest.qtechtheory.org/ (accessed 5 April 2022). [7] CIMdata, CIMdata Publishes Simulation and Analysis Market Report [website], 2021, https://www.cimdata.com/en/news/ item/16004-cimdata-publishes-simulation-and-analysis-marketreport (accessed 5 April 2022).

[8] J. Preskill, 'Quantum computing 40 years later', *arXiv*, 2021, pp.8-9. DOI: 10.48550/ARXIV.2106.10522.

[9] P. Byrne, 'Quantum Computing Without Qubits', *Quanta Magazine* [website], 2015, https://www.quantamagazine.org/ivan-deutschinterview-on-quantum-computers-20150122 (accessed 5 April 2022).

[10] E. Grumbling and M. Horowitz (eds.), *Quantum Computing: Progress and Prospects, Washington,* DC, The National Academies Press, 2019. ISBN: 978-0-309-47969-1.

[11] H. Kramer, 'ISS Utilization: CAL (Cold Atom Laboratory)', *eoPortal* [website], 2021, https://directory.eoportal.org/web/eoportal/satellite-missions/i/iss-cal (accessed 5 April 2022).

[12] Jet Propulsion Laboratory, *What We Do* [website], 2022, https:// coldatomlab.jpl.nasa.gov/what-we-do/ (accessed 5 April 2022).

[13] K. Frye et al., 'The Bose-Einstein Condensate and Cold Atom Laboratory', *EPJ Quantum Technology*, vol. 8, no. 1, 2021, p. 3. DOI: 10.1140/EPJQT/S40507-020-00090-8.

References and further reading

[14] Quantum Flagship, Quantum Technology | The future is Quantum[website], 2022, https://qt.eu/ (accessed 5 April 2022).

[15] M. Reynolds, 'Quantum simulator with 51 qubits is largest ever', New Scientist [website], 2017, https://www.newscientist.com/ article/2141105-quantum-simulator-with-51-qubits-is-largest-ever/ (accessed 5 April 2022).

[16] S. Ebadi et al., 'Quantum Phases of Matter on a 256-Atom
Programmable Quantum Simulator', *Nature*, vol. 595, no. 7866, 2021, pp. 227–232. DOI: 10.1038/S41586-021-03582-4.

[17] PASQuanS, PASQuanS [website], 2022, https://pasquans.eu/ pasquans/ (accessed 5 April 2022).

[18] QuEra, QuEra Computing Inc: Scalable quantum computing with neutral atoms [website], 2022, https://www.quera.com/ (accessed 5 April 2022).

[19] Pasqal, *Technology & Applications - PASQAL* [website], 2022, https://pasqal.io/technology/ (accessed 5 April 2022).

11.S.C.

[20] T. Maiden, 'How big is the logistics industry?', *FreightWaves* [website], 2020, https://www.freightwaves.com/news/how-big-isthe-logistics-industry (accessed 5 April 2022).

[21] Crunchbase, ColdQuanta - Crunchbase Company Profile & Funding [website], 2022, https://www.crunchbase.com/organization/ coldquanta (accessed 5 April 2022).

[22] Crunchbase, D-Wave Systems - Crunchbase Company Profile &
 Funding [website], 2022, https://www.crunchbase.com/organization/
 d-wave-systems (accessed 5 April 2022).

[23] Crunchbase, PASQAL - Crunchbase Company Profile & Funding [website], 2022, https://www.crunchbase.com/organization/pasqal (accessed 5 April 2022).

[24] Crunchbase, infinityQ Technology - Crunchbase Company Profile & Funding [website], 2022, https://www.crunchbase.com/ organization/infinityq-technology-inc (accessed 5 April 2022).

Contact information



Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU



www.qcshub.org





uknqt.ukri.org

