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Hybrid Quantum/Classical and Quantum Computing uptake in UK

Dr Stefano Mensa
HPC Applications Specialist

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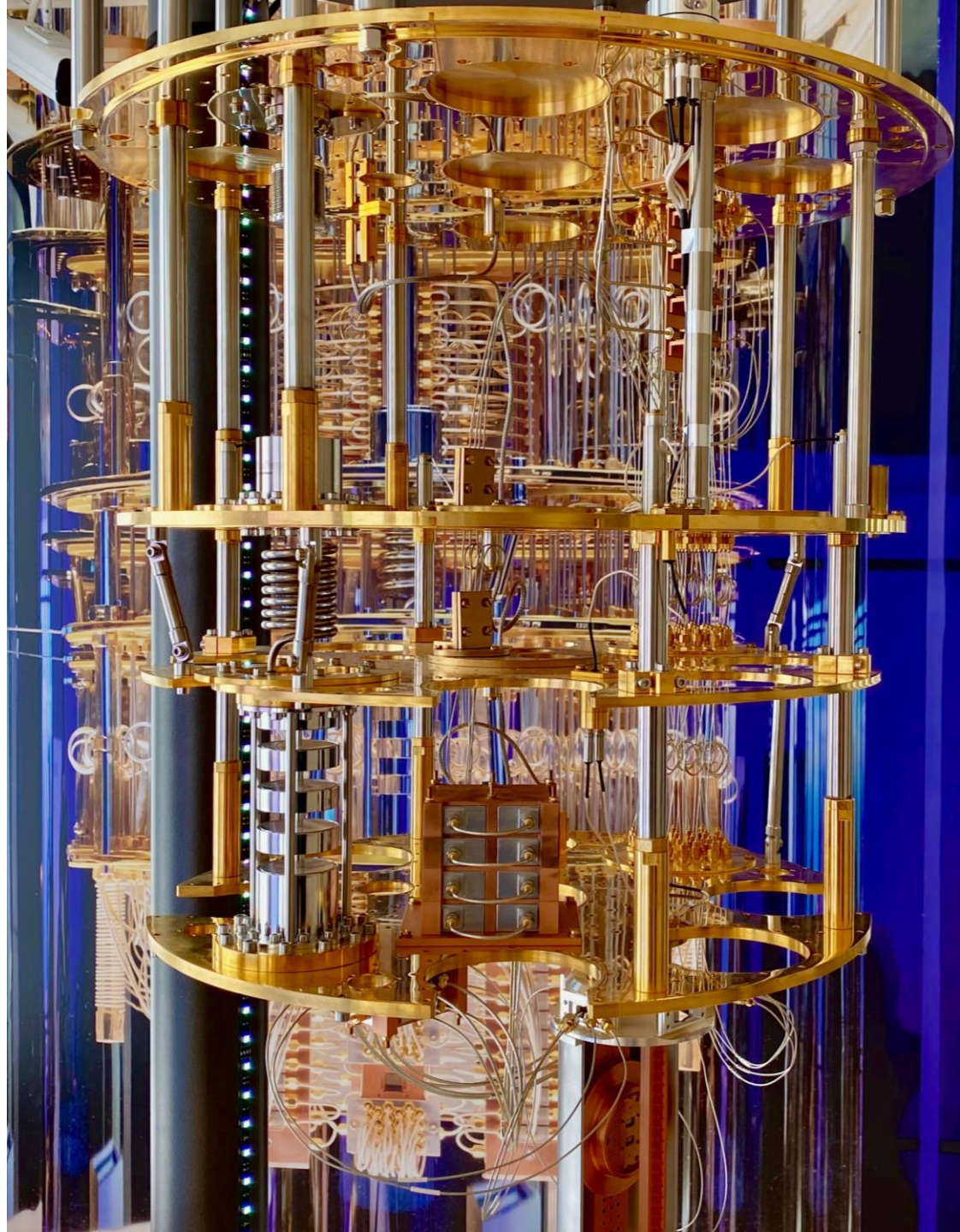
State of Quantum in 2022

1. HPC is alive and well
2. Quantum Computing is the future
3. Quantum needs HPC and *vice-versa*
4. HPC centres across the world are embracing Quantum. Are we ready for it?



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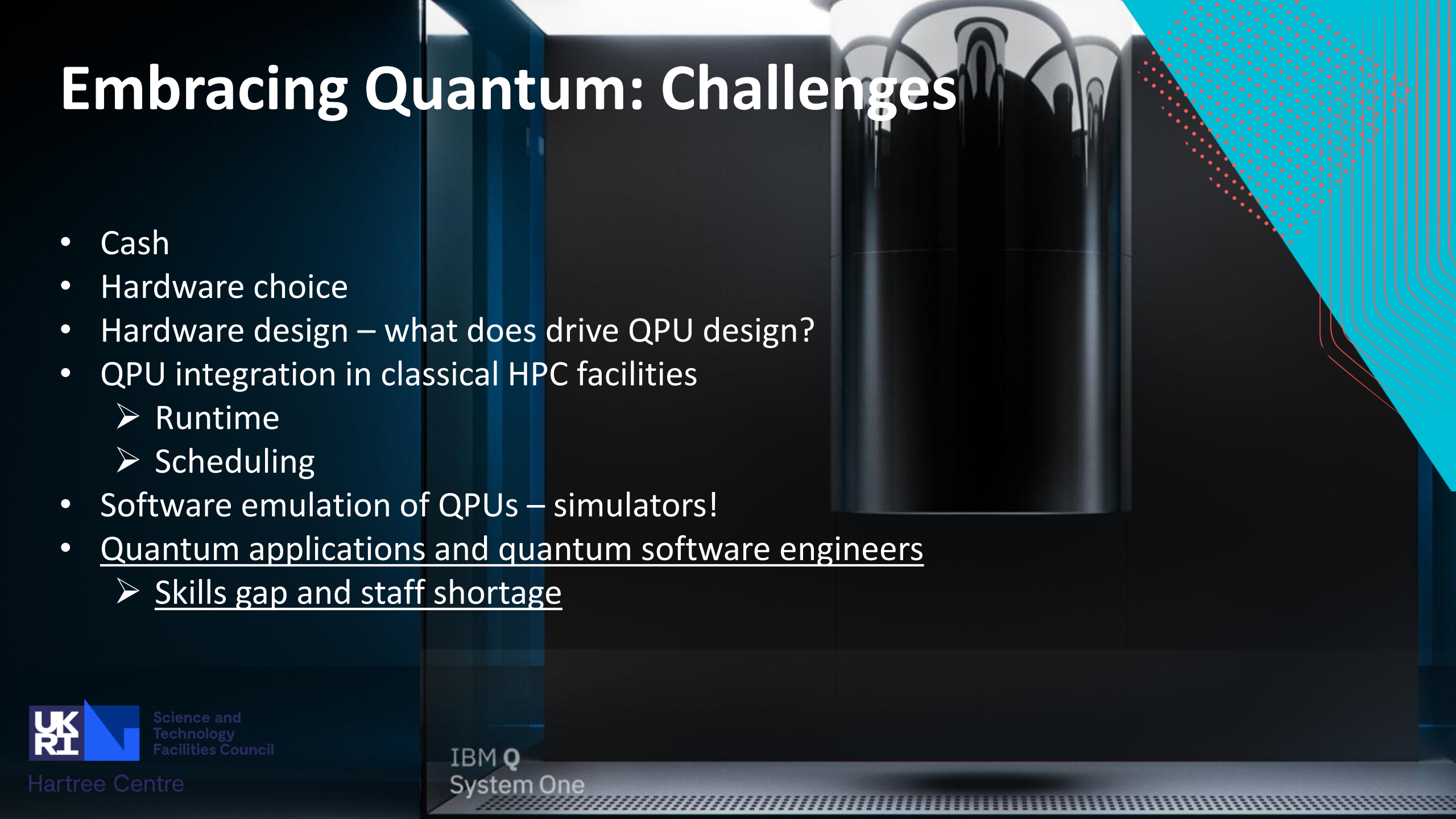
ISC High Performance
TRANSFORMING THE FUTURE

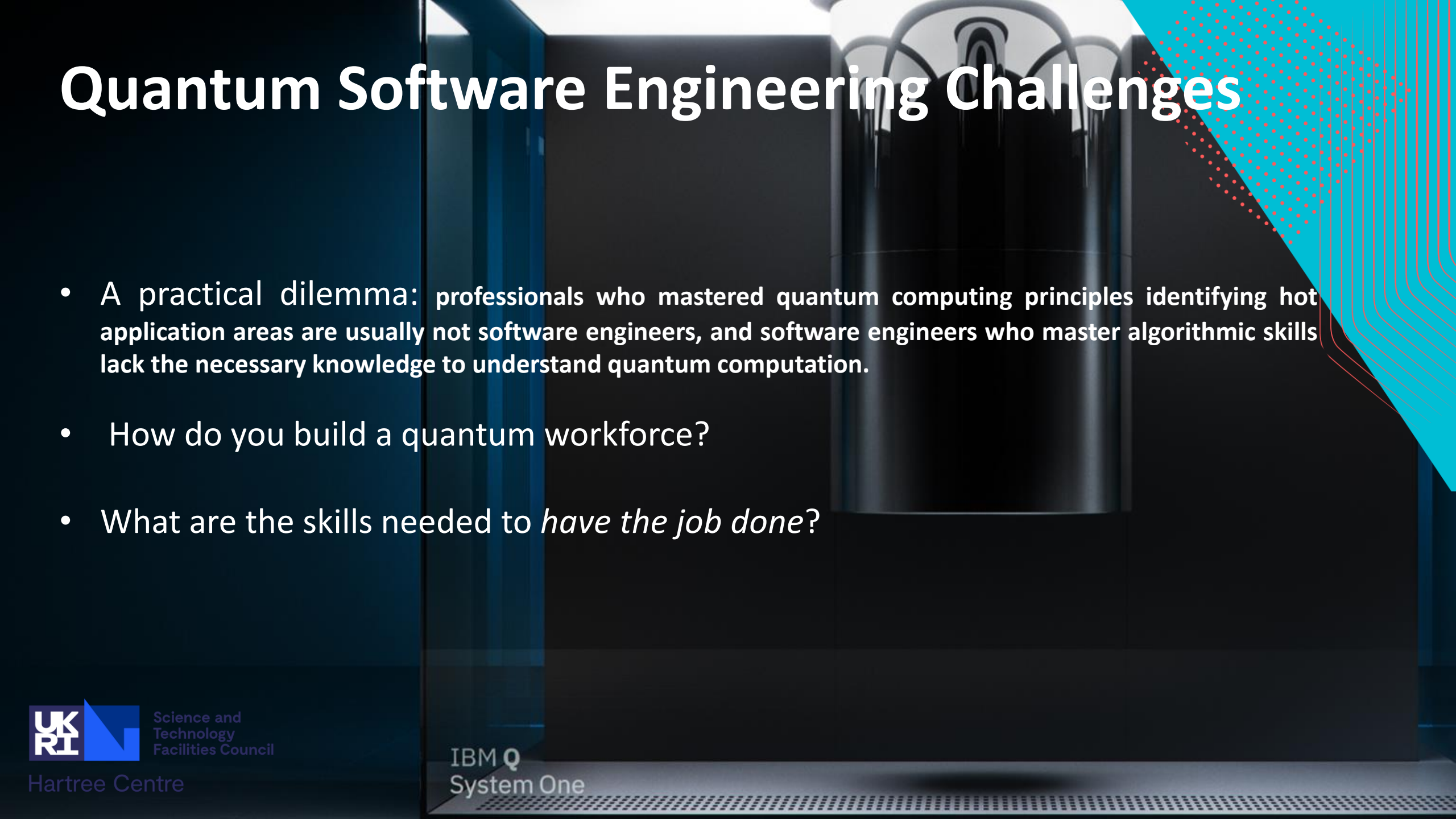
Embracing Quantum: Challenges

- Cash
- Hardware choice
- Hardware design – what does drive QPU design?
- QPU integration in classical HPC facilities
  - Runtime
  - Scheduling
- Software emulation of QPUs – simulators!
- Quantum applications and quantum software engineers
  - Skills gap and staff shortage



Quantum Software Engineering Challenges

- A practical dilemma: **professionals who mastered quantum computing principles identifying hot application areas are usually not software engineers, and software engineers who master algorithmic skills lack the necessary knowledge to understand quantum computation.**
- How do you build a quantum workforce?
- What are the skills needed to *have the job done*?



Hartree's Recipe to Quantum Uptake

- Funding opportunities and a quantum provider partner
  - Hartree National Centre for Digital Innovation
  - IBM Quantum
  - Access to the IBM aviary of quantum computers
- A meaningful asset of real-world case studies
  - Hartree aims at providing tangible benefits of quantum computing to UK's industrial sector.
  - Long standing portfolio of collaborations
- Staff willing to take the risk – upskill first, hire next

Hartree National Centre for Digital Innovation (HNCDI)

- New collaborative partnership with IBM Research £172M UK Govt investment + £38M IBM in-kind
- Enabling businesses and public sector organisations to adopt AI and quantum computing
- A dynamic and supportive expert environment for **UK organisations of all sizes** to explore the latest technologies, develop proofs-of-concept and apply them to industry and public sector challenges for **productivity, innovation** and **economic growth**.
- Helping navigate the possibilities, de-risk investment into new technologies and discover the next step

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Tackling industry challenges

Skills
Tackling gaps within your organisation and widening the talent pool

Technical Capability
Exploring and evaluating data-driven AI technologies to help enhance productivity

Application
Developing and implementing practical solutions within your business

Resilience
Knowing how to prepare for and when to invest in the right emerging technologies (e.g. quantum computing)

EXPLAIN

EXPLORE

EXCELERATE

EMERGING TECHNOLOGY

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Our track record

Quantum Uptake in Hartree Centre

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Routing Warehouse Robots

- A quantum/classical hybrid solver was applied to routing robots in Ocado's Customer Fulfillment Centers.
- Combining these two computing paradigms to produce a better solution than would be possible if used in isolation.
- After considering trans-Atlantic communication, quantum annealing approach starts to become competitive.

ocado TECHNOLOGY

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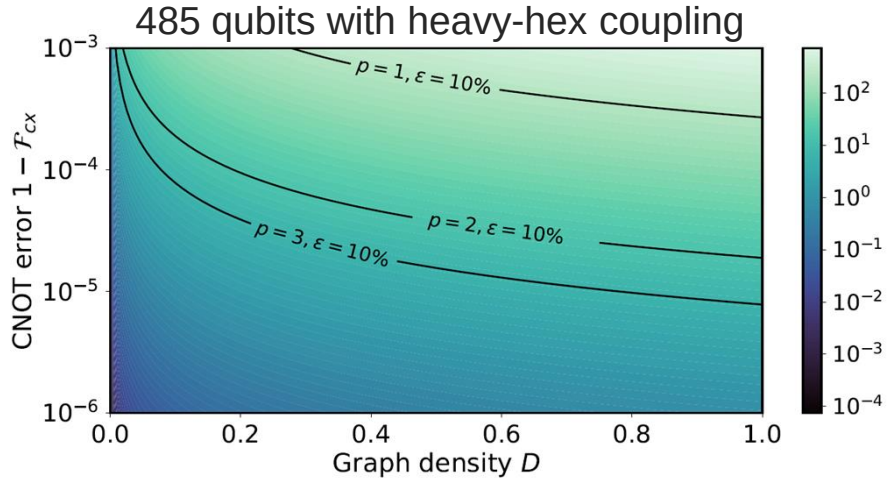
D:wave
The Quantum Computing Company™

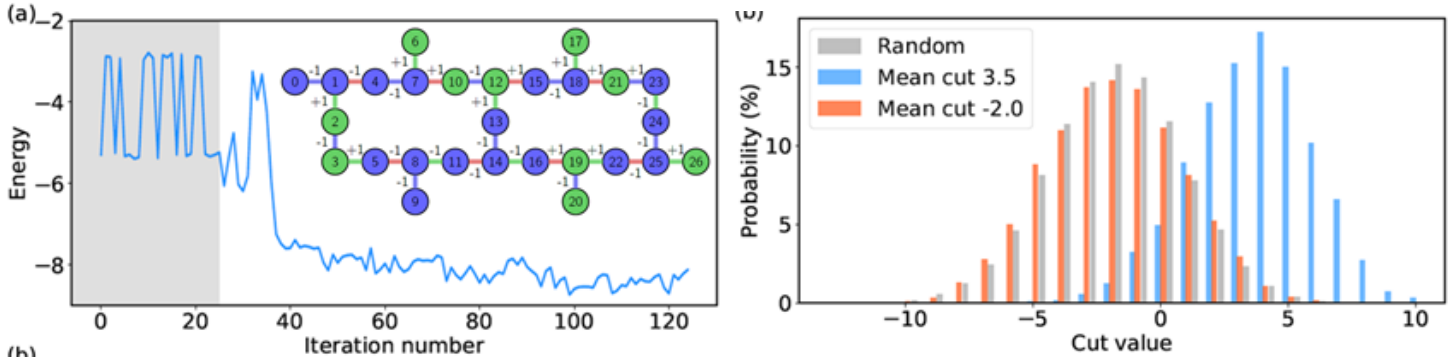
Quantum Optimization for Routing

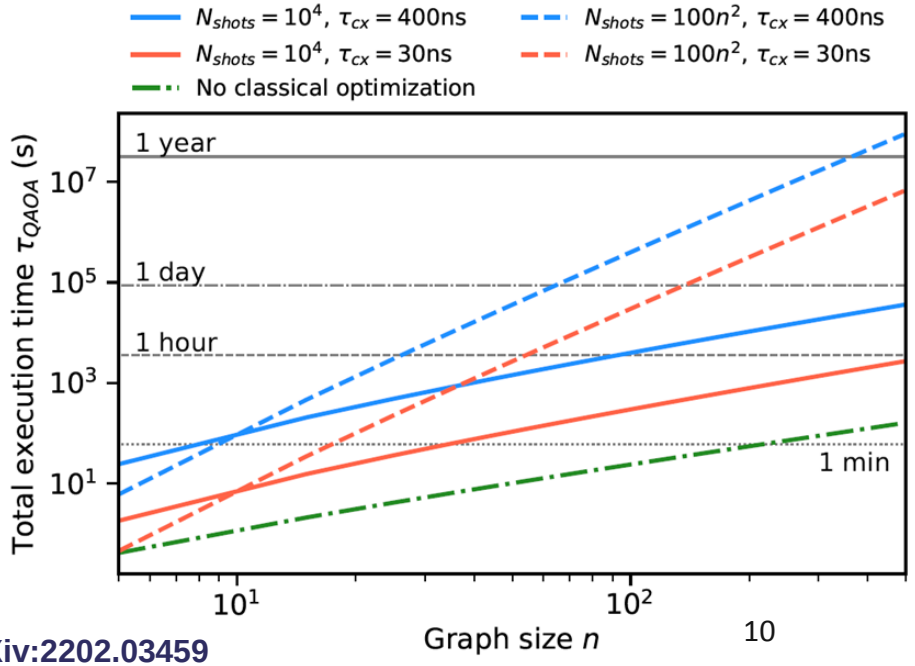
IBM **Quantum**

Team: Vendel Szeremi, Julien Gacon, Dariusz Lasecki, Daniel Egger, Luciano Bello, Stefan Woerner

- Developed SWAP strategies
  ⟹ Overcome limited device connectivity.
- Evaluated gate fidelity criteria for the SWAP strategies
  ⟹ When does it make sense to run on noisy hardware?
- Estimates of execution time on quantum hardware
  ⟹ Identify bottlenecks.
- Qiskit QAOA Runtime
  ⟹ Explore QAOA at scale.







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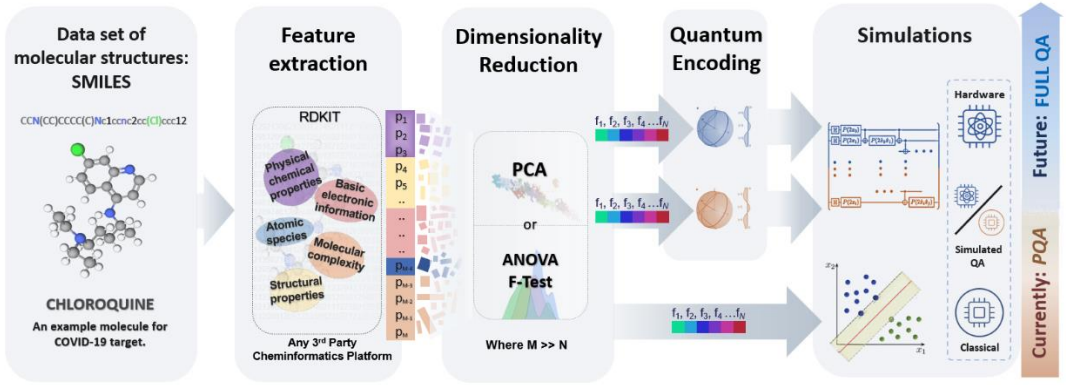
Paper: "Scaling of the Quantum Approximate Optimization Algorithm" **arXiv:2202.03459**

QML Framework for Virtual Screening in Drug Discovery

IBM **Quantum**

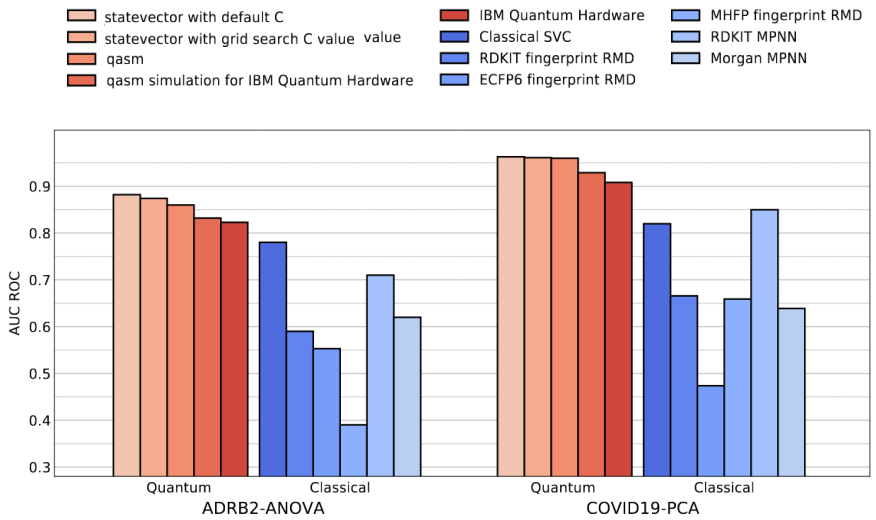
Team: Stefano Mensa, Emre Sahin, Francesco Tacchino, Panagiotis Kl. Barkoutsos, Ivano Tavernelli



Virtual screening: searching digital libraries of molecules to identify structures which are most likely to bind to a drug target.

Prospective Quantum Advantage: we observe instances in which simulated quantum algorithms and proof-of-principle hardware experiments on a reduced number of features outperform classical methods in the same conditions. No evident restrictions to the extension to larger problem sizes.

- Interface QML functionalities in Qiskit with cheminformatics tools (RDKit): automated and integrated workflow
- Investigate a novel practical use of quantum kernel methods using classical molecular data/descriptors
- Assess the potential for quantum advantage, supporting it with empirical evidence
- Experiments (8 qubits) on IBM Quantum Montreal and Guadalupe
- Contribution to Qiskit Nature and ML



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Paper: "Quantum Machine Learning Framework for Virtual Screening in Drug Discovery: a Prospective Quantum Advantage", arXiv:2204.04017

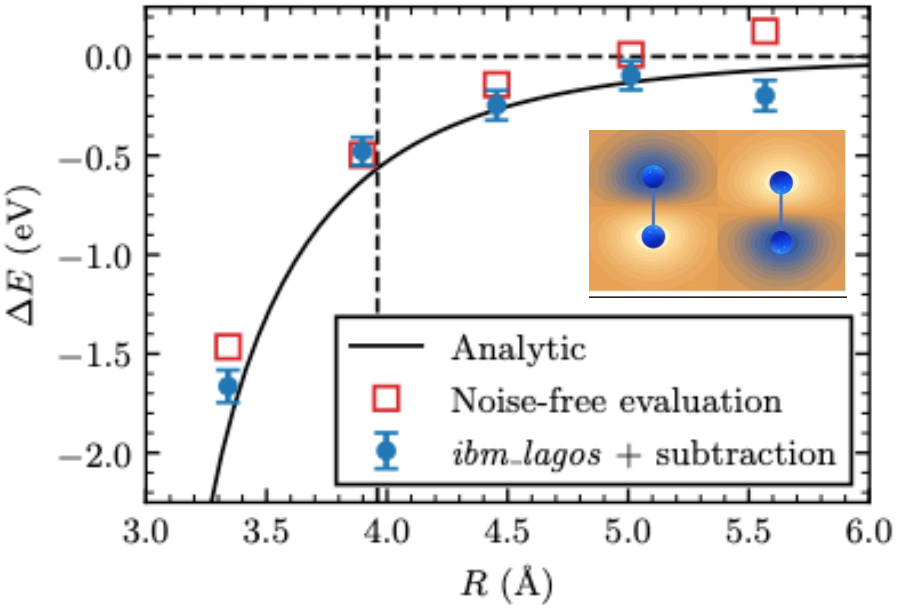
Weak intermolecular interactions on quantum processors

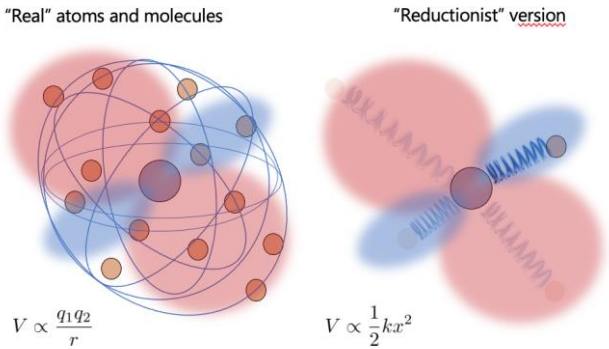
Team: Lewis W. Anderson, Martin Kiffner, Panagiotis Kl. Barkoutsos, Ivano Tavernelli, Jason Crain, Dieter Jaksch

- We developed a coarse-grained representation of the electronic response that is ideally suited for determining the ground state of weakly interacting molecules using a VQA.

➔ qubit resource grows linearly with the number of molecules

- We derived scaling behaviour for the number of circuits and measurements required, which compare favourably to traditional variational quantum eigensolver methods.
- Demonstrated on IBM hardware
- Corresponding Qiskit module in preparation





London Dispersion Forces: weak, non-covalent, molecular interactions which are particularly difficult to capture ab-initio using conventional electronic structure methods such as DFT.

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Paper: "Coarse grained intermolecular interactions on quantum processors", Physical review A (in press, 2022).

Non-HNCDI Funded Activities

Projects funded by Commercialising Quantum Technologies: CRD & Tech round 2

QuPharma: The consortium lead by SeeQC will build and deliver a full-stack quantum computer for pharmaceutical drug development. The QuPharma project will enable the UK to build a commercially scalable application-specific quantum computer designed to tackle prohibitively high costs and dramatically reduce the time required for drug development on a global scale. Collaboration including NQCC and STFC's Scientific Computing alongside Hartree.

QEC: The Quantum Error Correction (QEC) consortium includes end-user Rolls-Royce supported by the Science and Technology Facilities Council (STFC) Hartree Centre, quantum software developer Riverlane, supply chain partners Edwards, TMD Technologies (now acquired by Communications & Power Industries (CPI)) and Diamond Microwave, commercialisation and dissemination experts Sia Partners and Qureca and world-class academic groups from Imperial College London and the University of Sussex.

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Questions?