Grand Challenges

Collaborative Computational Project Quantum Computing (CCP-QC)

Over the next five to ten years, CCP-QC will align with the goal of the UK National Quantum Strategy Mission by supporting and developing the commercial provision of quantum computing as a service and their integration into high performance computational workflows, to have accessible quantum computers capable of running 1 trillion operations by 2035

The Community

www.ccp-qc.ac.uk

CCP-QC brings together close co-operation between other CCPs and the quantum computing community, rather than build a separate community for quantum computing. Encompassing members interested in enhancing their simulations by adding quantum computing capability to their code, as well as researchers working on applications of quantum computing to simulations, CCP-QC generates projects and develops methods appropriate to specific applications, leading to proof-of-concept demonstrations on early quantum hardware. They also have a partnership with the National Quantum Computing Centre (NQCC) in developing early applications of quantum computing, providing training and supporting career development. CCP-QC promotes cross-CCP networking to share knowledge on early applications of quantum computing, enabling the widest possible early adoption of quantum enhanced computational science, collaborating with industry and partners who are key players in developing quantum computing technology both in the UK, and internationally.

The Challenge

To support the UK Strategy by demonstrating quantum assisted computation, developing enhanced algorithms and workflows

The UK National Quantum Strategy Missions set out by government in 2023 lists five missions for quantum technology to deliver over the next ten years. The relevant mission for quantum computing is Mission One: **By 2035, there will be accessible, UK-based quantum computers capable of running 1 trillion operations and supporting applications that provide benefits well in excess of classical supercomputers across key sectors of the economy.** Crucially, this will be achieved not only by supporting commercial provision of quantum computing as a service, but also by seamlessly integrating quantum computing into high performance computational workflows, enabling user access and widespread adoption. High impact will be achieved in the following sectors at a minimum: healthcare, finance, transport, defence, energy, and manufacturing. The missions specify milestones towards the 2035 capability. For Mission One:

• By 2028, extending beyond the NISQ-era with a million quantum operations, which will enable the exploration of applications associated with the simulation of chemical processes, helping to improve catalyst design, for example.

• By 2032, demonstrating large-scale error correction capabilities with a billion quantum operations, with applications including accelerated drug discovery.

• By 2035, achieving quantum advantage at scale through reaching a trillion quantum operations, enabling applications such as optimising the production of clean hydrogen.

Ensuring that scientific advances in quantum computing applications can be applied with confidence in both industry and the public sector requires "real-world engineering utility" - industrial companies running reliable quantum computing to improve their designs. Part of this requires quantum computing to meet any accuracy requirements from regulatory bodies. In much of engineering (especially aerospace and civil/structures) there are strict design regulations, and quantum computing will need to work within legal frameworks and standards. The potential legal barrier of integrating quantum into mainstream engineering compute (e.g. helping to design a plane) has not yet been considered in detail.

The Solution

To enable early adoption of quantum computing in the workflows of CCPs and HECs

The first milestone - useful chemical and materials science calculations assisted by quantum computing - is just two years ahead. Thus, the first grand challenge for CCP-QC is to demonstrate useful quantum assisted computation for a specific industrially-relevant application within the domain of chemistry and materials science. This will require partnership with the relevant CCPs, HECs (CCP5, CCP9 and MCC) and the STFC Compute team, to enable early adoption of quantum computing in the workflows to deliver useful results. Two years from now is very ambitious, but CCP-QC are building on collaborations which began in 2019, with useful algorithms and workflows at their disposal from research funded under the ExCALIBUR programme and the CCP Bridge projects. With further resources, and in collaboration with other players, including the NQCC and QCi3 Quantum Tech Hub, this grand challenge is achievable. The next milestone is just four years after 2028: with larger quantum computers it will be possible to scale up to biomolecules. Collaboration with CCPBioSim will be critical to achieving meaningful, useful results. Alongside this, if CCP-QC are to achieve useful quantum computing enhanced workflows in other application areas besides quantum simulation, they will start working now to develop the algorithms and workflows ready for large scale quantum computers in 2035. The community already have an established collaboration and network for fluid simulations, and some of the methods can be expected to be more widely applicable for differential areas. More general applications have also been developed as part of the ExCALIBUR programme and need to be tested for future deployment as integrated hardware becomes available.

The Outcome

Ensuring that scientific advances in quantum computing applications can be applied with confidence in both industry and the public sector

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CCP-QC has already developed quantum accreditation - an efficient classical scheme of determining the correctness of real-world quantum computations. This scheme does not rely on performing an exponentially expensive classical simulation of the relevant quantum computation. NPL is one of their key collaborators and is already working on standards for quantum computing. There is much more to be done beyond their current focus, working with application communities to develop ways to certifying quantum computing efficiently against relevant standards and regulations, and to update regulations where necessary to allow future use of quantum computing.

More Information

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