Science and Technology Facilities Council

Hartree Centre

Using quantum computing to improve molecular modelling in drug development

STFC Hartree® Centre worked with AstraZeneca and Algorithmiq through the Hartree National Centre for Digital Innovation (HNCDI) programme to improve molecular modelling accuracy and accelerate drug development.

Challenge

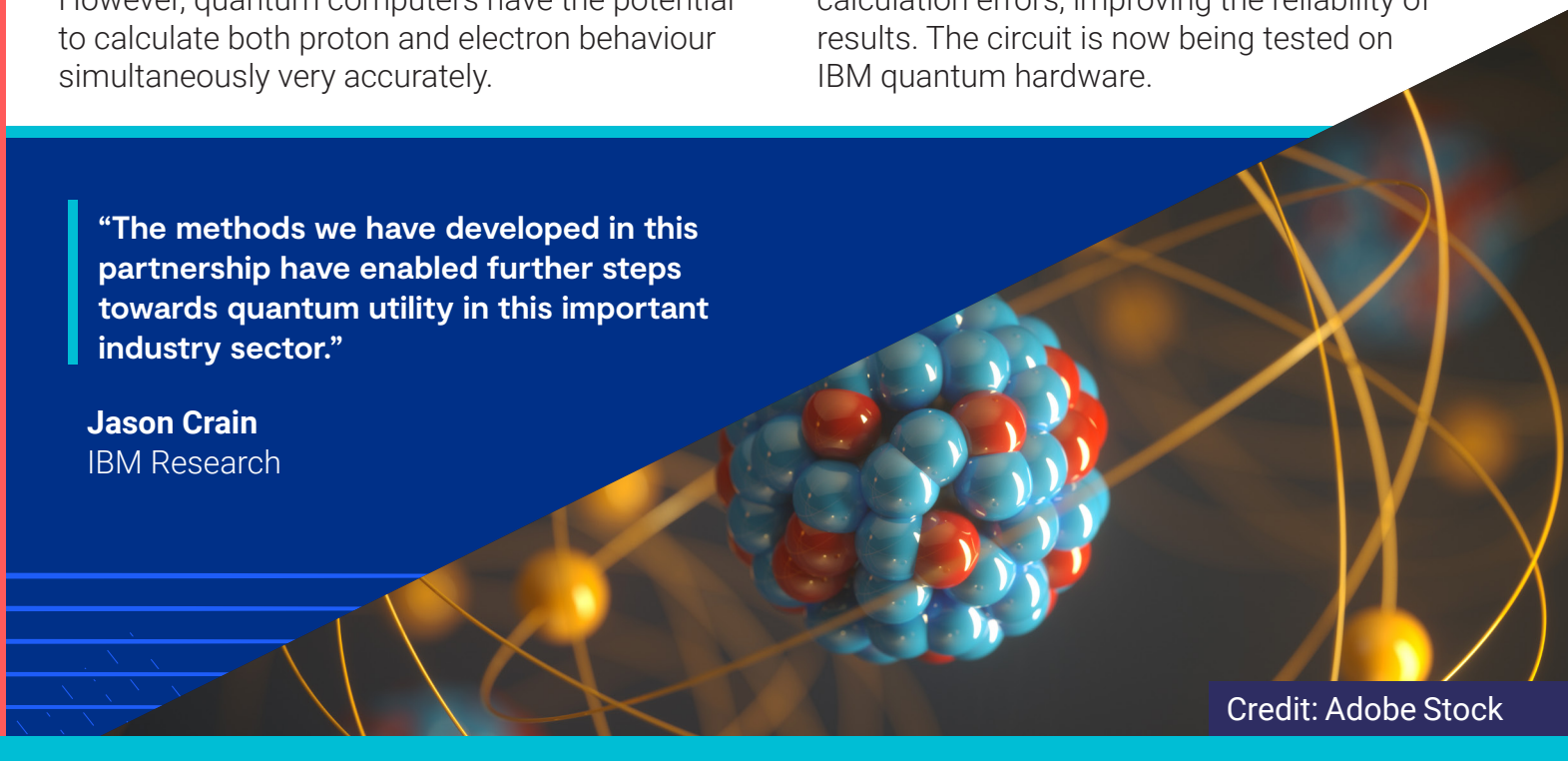
Drug discovery and development is time-consuming, taking on average 10-15 years from drug discovery to market. Computational modelling of reaction pathways and mechanisms can help facilitate the synthesis of drug candidates and accelerate the development of new medicines for patients. To achieve this, we must understand how potential drug candidates behave at a molecular level by modelling interactions between protons and electrons. Because these components are so chaotic and rapid, modelling this accurately is resource-intensive, and currently only the movement of electrons is calculated, whereas proton behaviour is approximated. This reduces the quality and precision of collected data. However, quantum computers have the potential to calculate both proton and electron behaviour simultaneously very accurately.

Approach

Through the HNCDI programme, the Hartree Centre and IBM worked with global biopharmaceutical company AstraZeneca to utilise quantum computing. AstraZeneca developed a quantum computing framework that characterises both protons and electrons accurately. The team then collaborated to refine and optimise a quantum circuit capable of modelling the coupled electron-proton dynamics. Initially, the circuit was resource-intensive and too complex to fit into the current available hardware. The team sought assistance from Algorithmiq to improve on this by streamlining the circuit and significantly reducing its resource requirements. This collaboration also enabled more efficient data analysis by reducing calculation errors, improving the reliability of results. The circuit is now being tested on IBM quantum hardware.

> **"The methods we have developed in this partnership have enabled further steps towards quantum utility in this important industry sector."**

Jason Crain
IBM Research



Credit: Adobe Stock

Benefits

A more accurate characterisation of molecular interactions involved in drug synthesis will enable more efficient development of drug candidates going forward, saving time, resources and costs. Overcoming the challenge of modelling proton and electron behaviour represents a significant scientific advancement. It pushes the boundaries of computational capacity and demonstrates scalability in quantum computing frameworks, opening new avenues for innovation and problem-solving.

At a glance

- Leveraging quantum computing to produce accurate and precise representation of molecular dynamics.
- Significant reduction of resource requirement when simulating molecular dynamics.
- Demonstration of quantum computer capacity and scalability.
- Deep insights to accelerate decision making during drug synthesis, saving time, resources and reducing costs in pharmaceutical research and development.

Who we are

The Hartree Centre was created by UK Government to help businesses and public sector organisations accelerate the adoption of high performance computing (HPC), big data analytics, artificial intelligence (AI) and quantum technologies. We play a key role in realising UK Government's Industrial Strategy by stimulating applied digital research and innovation, creating value for the organisations we work with and generating economic and societal impact for the UK. We are proud to be part of UK Research and Innovation.

What we do

- Boost productivity and innovation for industry
- Offer training and skills development
- Provide insights into future technologies
- Give tailored business development support
- Build bespoke small teams around your project