Science and Technology Facilities Council

Hartree Centre

Boosting the efficiency of drug discovery using quantum computing

As part of the Hartree National Centre for Digital Innovation (HNCDI) programme, STFC Hartree® Centre collaborated with IBM Research to explore how quantum computing can be used to increase efficiency in drug discovery and development.

Challenge

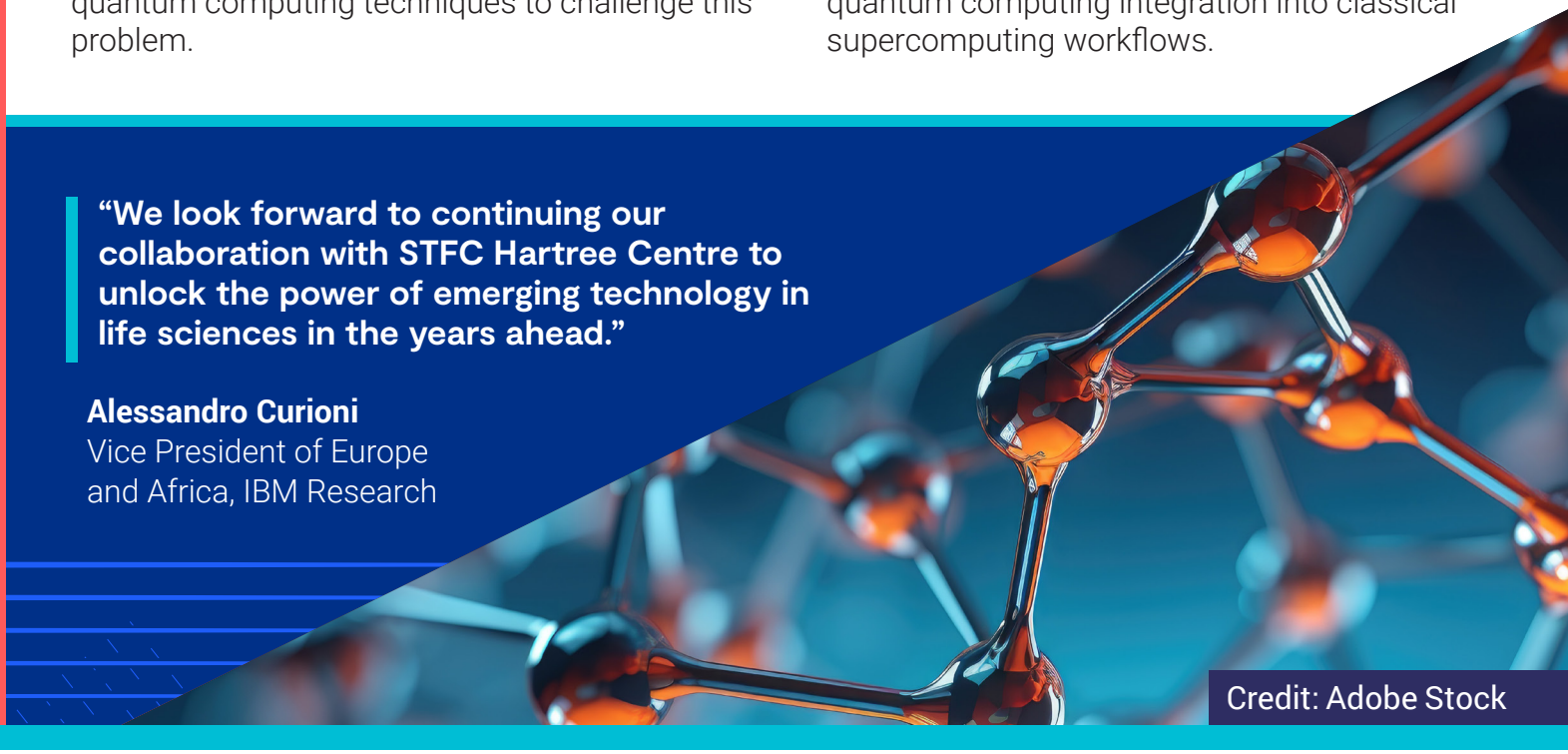
Early drug discovery processes are notoriously expensive and time-consuming. First, a compound that could work as a drug candidate has to be identified. This involves searching a computer database and comparing different molecules with unknown activity to a drug target to see which is the most compatible. This drug candidate must then be tested through laboratory experiments to determine its potential for success as a drug. There is an incredibly high failure rate, as many drug candidates identified in this early phase are unsuccessful in further testing and development. This means that drug discovery and development is not only a time-consuming, costly process, but it is also a risky one for stakeholders as many investments fail. Our team leveraged cutting-edge quantum computing techniques to challenge this problem.

Approach

In collaboration with IBM, our team proposed the integration of quantum computing into a classical computing workflow for drug discovery. A quantum computer was used to train a machine-learning algorithm that identifies a drug candidate from the database. By introducing the quantum training to this workflow, the team were able to boost the accuracy of identification significantly compared to existing classical techniques. This results in a stronger set of candidates that are more likely to be successful throughout the drug development process. This shows the potential advantage of quantum computing for the pharmaceutical industry, whilst also demonstrating the concept of seamless quantum computing integration into classical supercomputing workflows.

> **"We look forward to continuing our collaboration with STFC Hartree Centre to unlock the power of emerging technology in life sciences in the years ahead."**

Alessandro Curioni
Vice President of Europe and Africa, IBM Research



Credit: Adobe Stock

Benefits

The team were able to find potential improvements in identification accuracy, in some cases of as much as 20%, with expectations that quantum computers will scale and be integrated into the classical workflow. By improving the identification accuracy of prospective drug candidates, the time and cost of the drug discovery and development process can be significantly reduced. Additionally, increased identification accuracy mitigates investment risk for stakeholders by ensuring resources are directed to the most promising candidates. The successful integration of quantum computing into the drug discovery workflow paves the way for accelerated advancements in pharmaceutical research and suggests the potential for broader applications of quantum computing across diverse industries.

At a glance

- Mitigated risk of failure in drug discovery and development.
- Quantum computing is capable of surpassing classical methods, enhancing drug candidate classification accuracy.
- Seamless integration of quantum computing into classical computing workflow.
- Demonstration of the capabilities of quantum computing in the face of large, complex data sets.

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