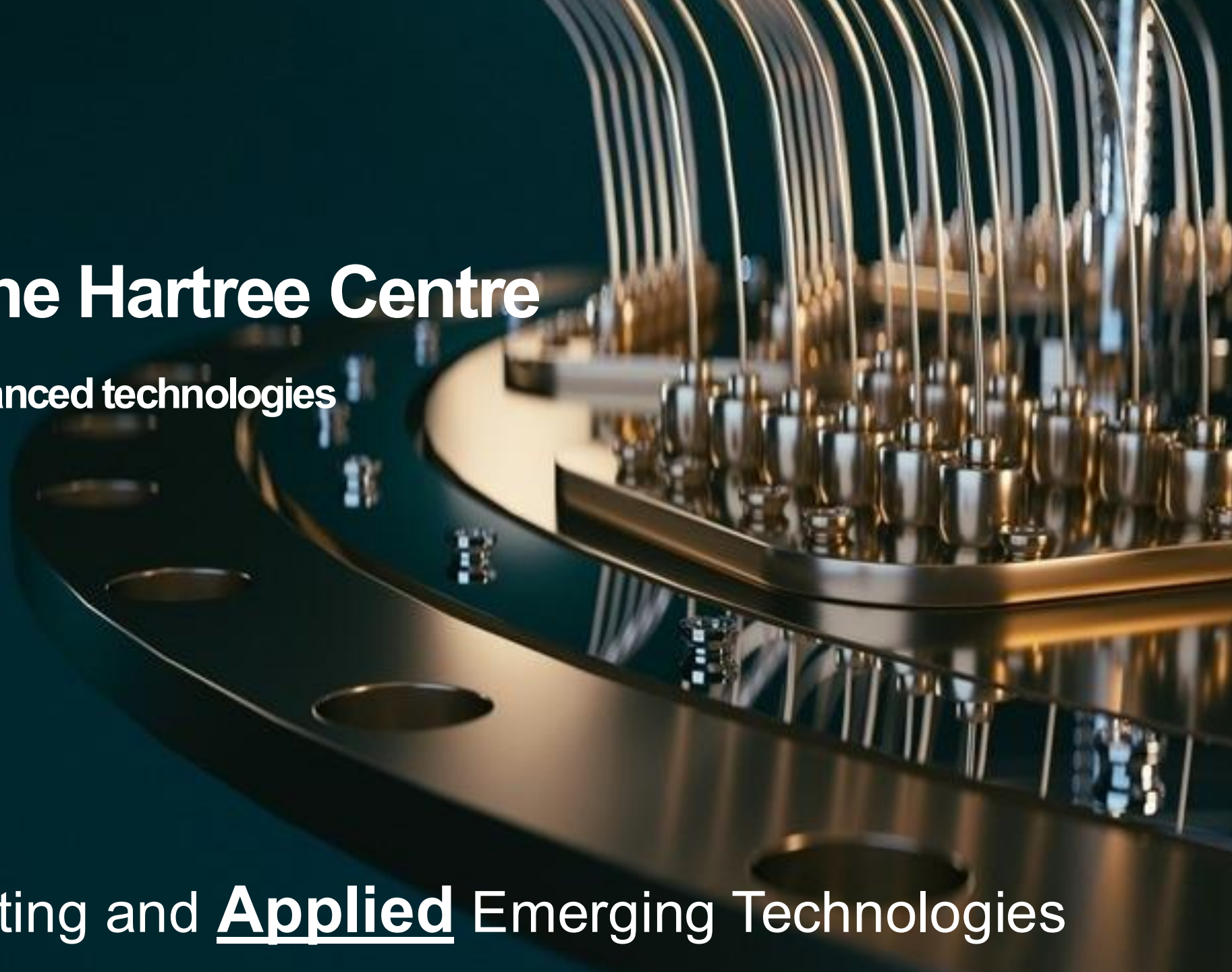
Science and Technology Facilities Council

Hartree Centre



Quantum At The Hartree Centre

The Convergence of advanced technologies

Getting Quantum Right

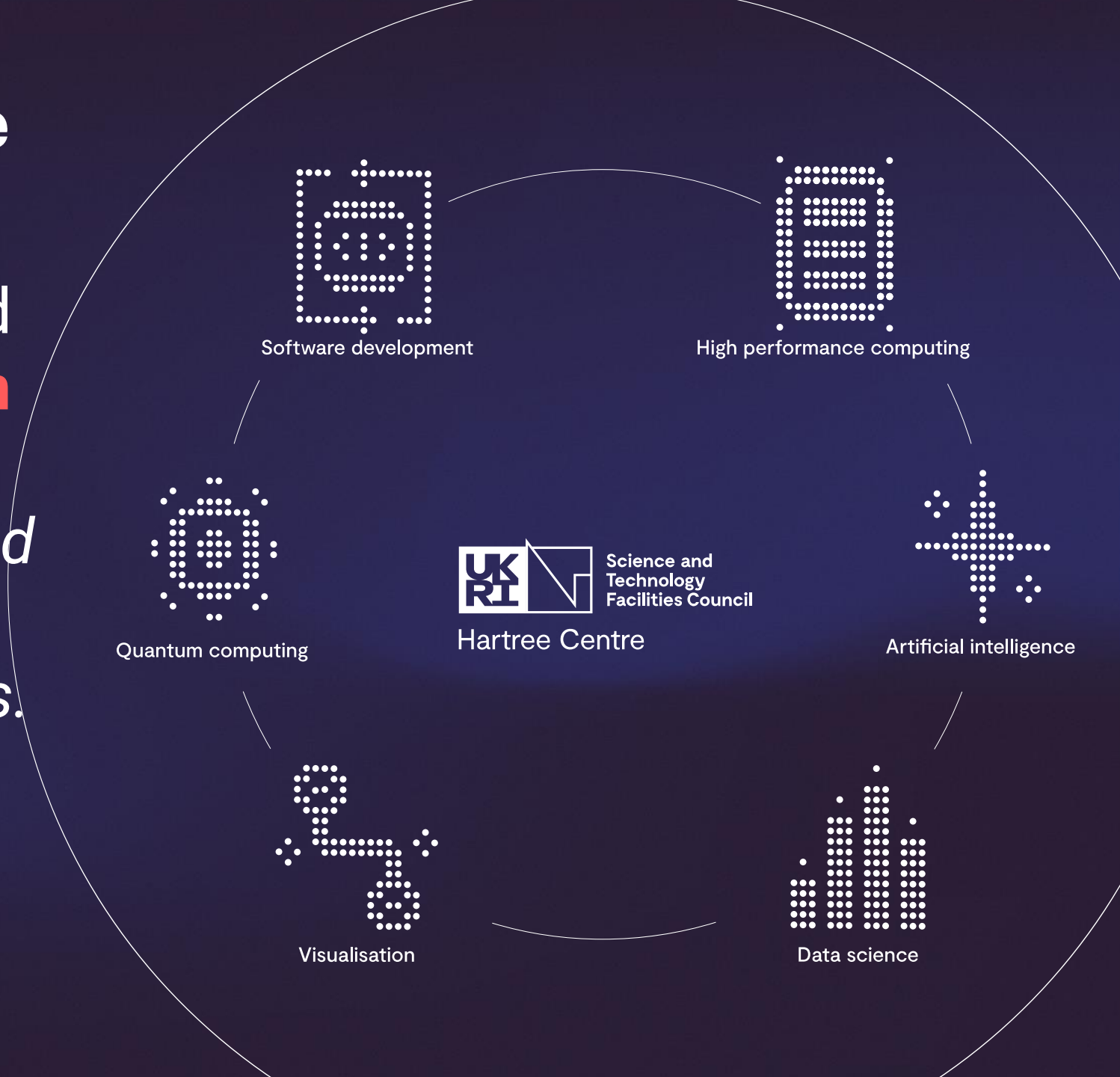
Partnerships

Case Studies

Advanced Computing and **Applied** Emerging Technologies

What makes us unique

The Hartree Centre is uniquely positioned to lead the **datacentric integration** of QC - *leveraging its expertise, infrastructure, and partnerships to build next generation digital platforms.*



Science and Technology Facilities Council
Hartree Centre

Facts and figures

174
Full time employees

900
Organisations

9360
Individuals trained

150
Completed projects

15
Platforms

300+
Industry collaborators

10
Patents

60
Peer reviewed papers

50
Open-source assets

£27M
Operational budget

Science and Technology Facilities Council
Hartree Centre

HNCDI

Hartree National Centre for Digital Innovation

IBM

550+
Organisations engaged

£4.7m+
Cost savings for organisations

£832m+
Net present value

% of organisations reported:

83%
Very satisfied

74%
Productivity gains

57%
Efficiency gains

78%
Improved brand value

The Hartree National Centre for Digital Innovation

2022-2026

6

Advanced Computing & Emerging Technology Team

20+
Organizations engaged

30+
Peer Reviewed Articles

5
Open-Source Projects

4
Global Working Groups Steered

1M+ ca.
Downloads

600+
Citations

12+
Workshops and Tutorials

600+ DSIT Staff on Training Courses

IEEE QTC Distinguished Synergy Award

£210M

A public-private partnership between UKRI and IBM to de-risk, develop and deploy HPC, AI and emerging technologies at scale.

150+
Projects

- Including 30+ projects involving **practical adoption of quantum computing** in industry applications.
  - ✓ Quantum-Centric Supercomputing
- **3+ Early-stage application projects of neuromorphic computing.**

£800M+

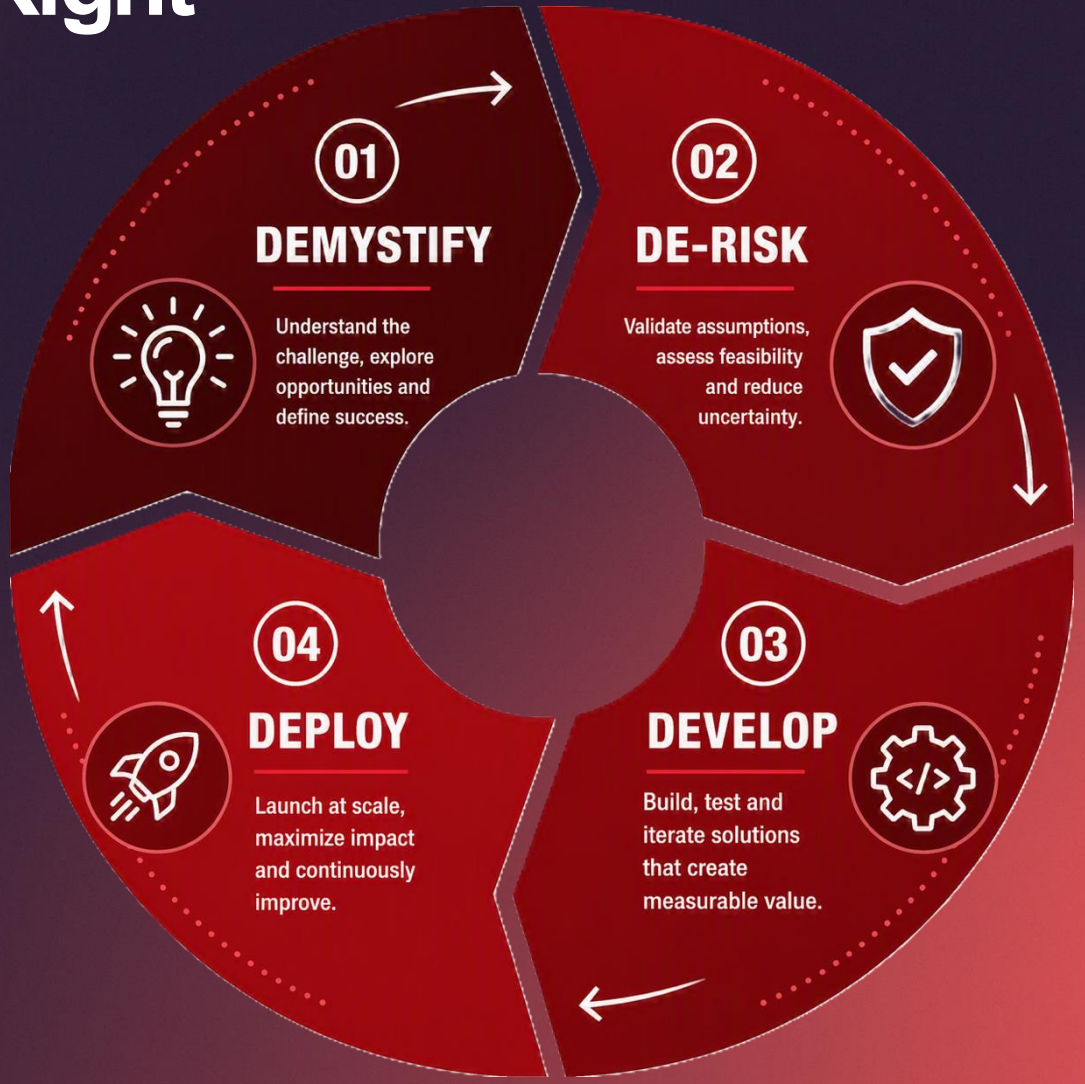
in **Net Present Social Value** estimated since 2022.

UKRI Science and Technology Facilities Council
Hartree Centre

IBM

Getting Quantum Right

Science and Technology Facilities Council
Hartree Centre



To equip UK industry with the knowledge, skills and compute needed to fully unlock the potential of quantum computing

Building the Quantum Ecosystem

Industry

AstraZeneca
algorithmiq
CGA SIMULATION
NHS
Rolls-Royce
ocado
AWE NUCLEAR SECURITY TECHNOLOGIES
e·on
QINETIQ
NATIONAL NUCLEAR LABORATORY
Cleveland Clinic
Transport for Greater Manchester

Research Partners

Lawrence Livermore National Laboratory
OAK RIDGE National Laboratory
CERN
USRA
KIT Karlsruher Institut für Technologie
DESY.

QSL Quantum Software Lab

THE UNIVERSITY of EDINBURGH
UNIVERSITY OF CAMBRIDGE
UNIVERSITY OF LIVERPOOL
UNIVERSITY OF OXFORD
IMPERIAL
UCL

UKRI Science and Technology Facilities Council
Hartree Centre

The Hartree Centre Quantum Agenda

f **Quantum Technical Expertise/Advisory:**

stics and **supply chain –** optimisation problems and scalability **.**

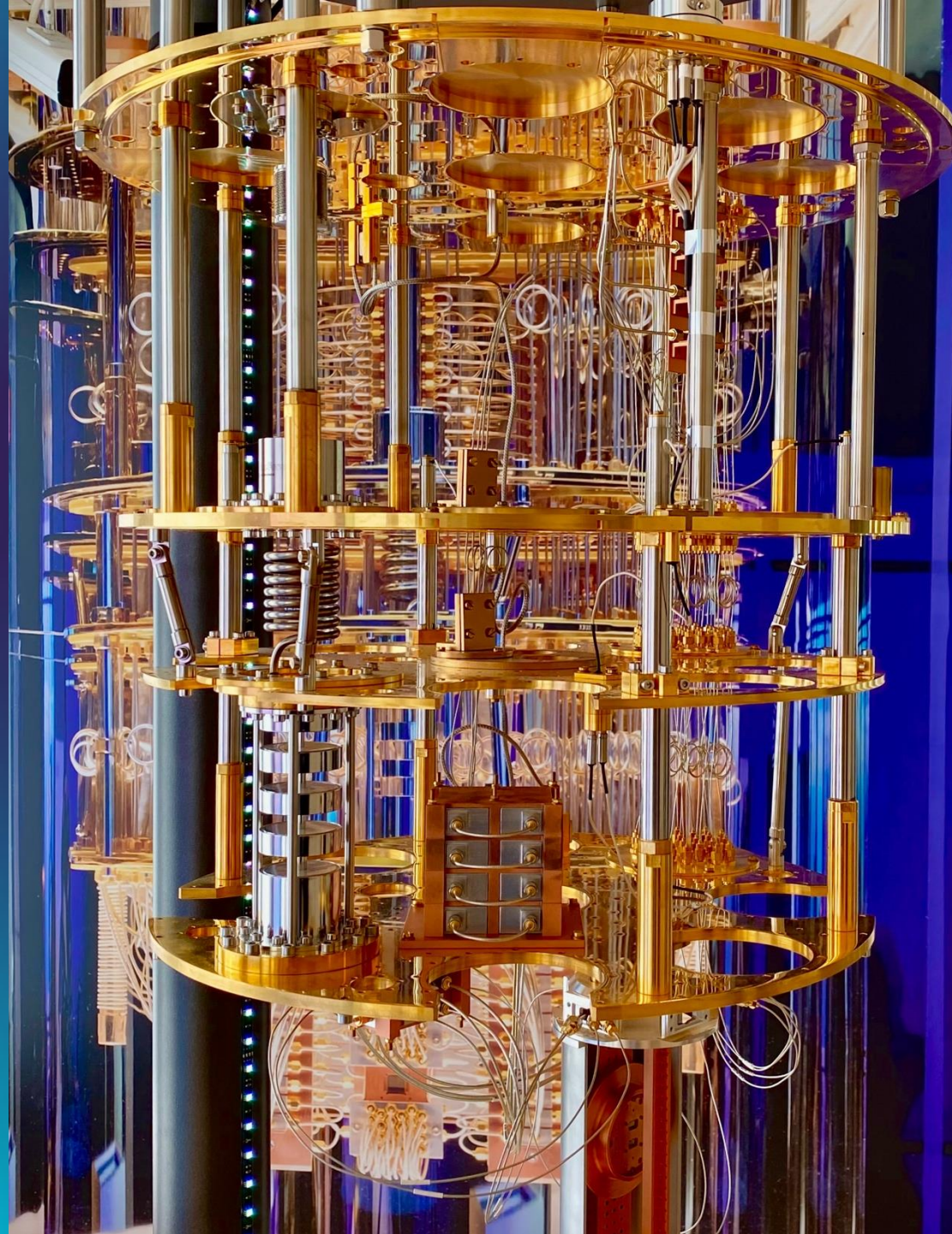
mistry and **Materials –** simulations, discovery.

neering – plasma physics, CFD, PDEs.

ntum Machine Learning – benchmarking and dards.

thcare and **Life Sciences –** Early Stages Drug overy, protein folding, computational histopathology.

nce and
nology
ities Council



Quantum Hardware and Software Partners

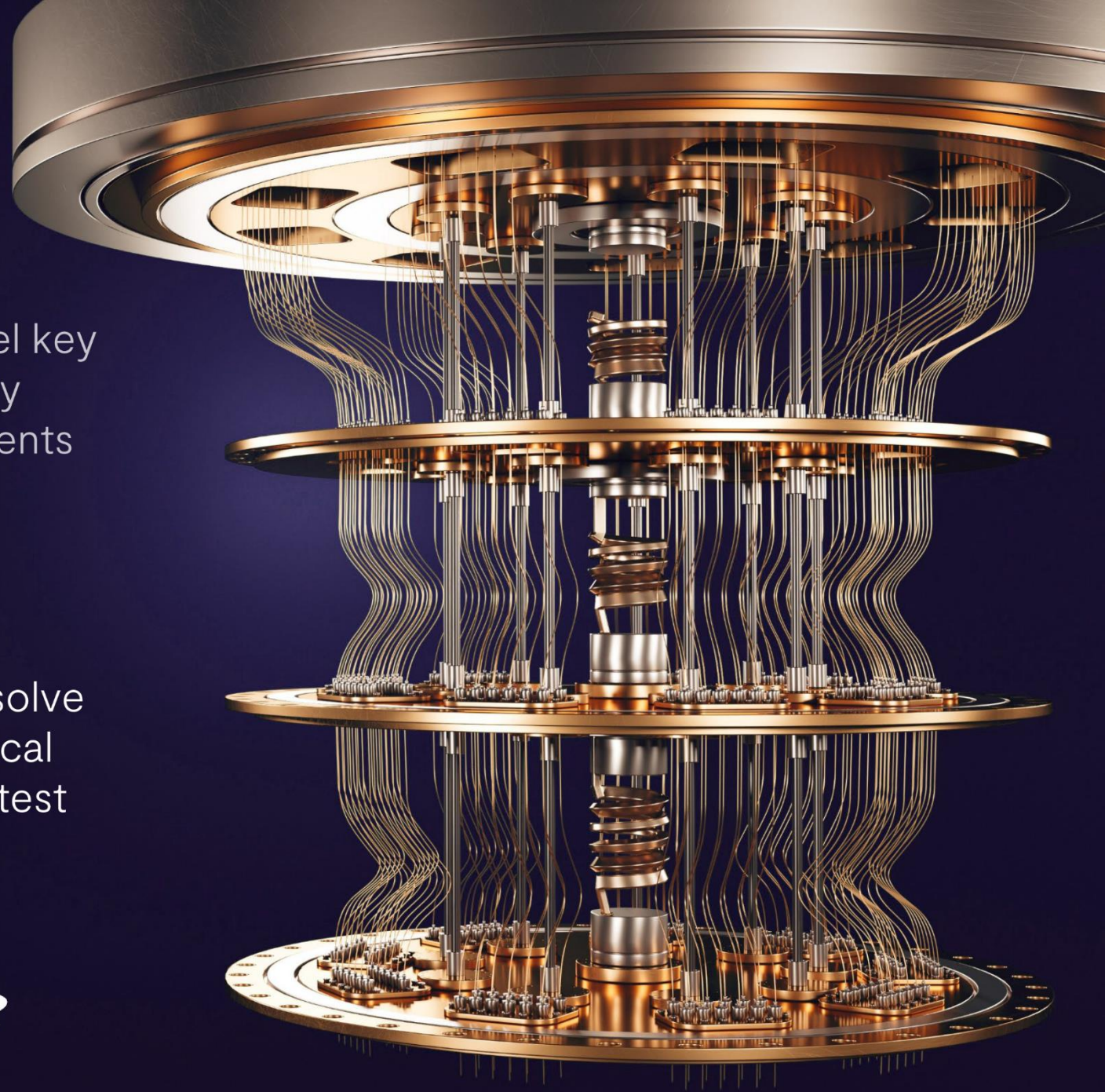
Hartree Centre

Challenge

Classical computing can't accurately model key drug discovery processes, leading to costly trial-and-error and slower progress to patients

Our impact

Partnered with AstraZeneca and IBM to identify where quantum computing could solve accuracy-limited problems in pharmaceutical R&D, prioritising applications with the greatest potential to accelerate drug development



UKRI Science and Technology Facilities Council
Hartree Centre

IBM

AstraZeneca

Challenge

Cancer slide images are large and computationally difficult to analyse quickly and accurately

Our impact

We improved cancer classification by using quantum machine learning to deliver faster analysis while reducing data and computational requirements

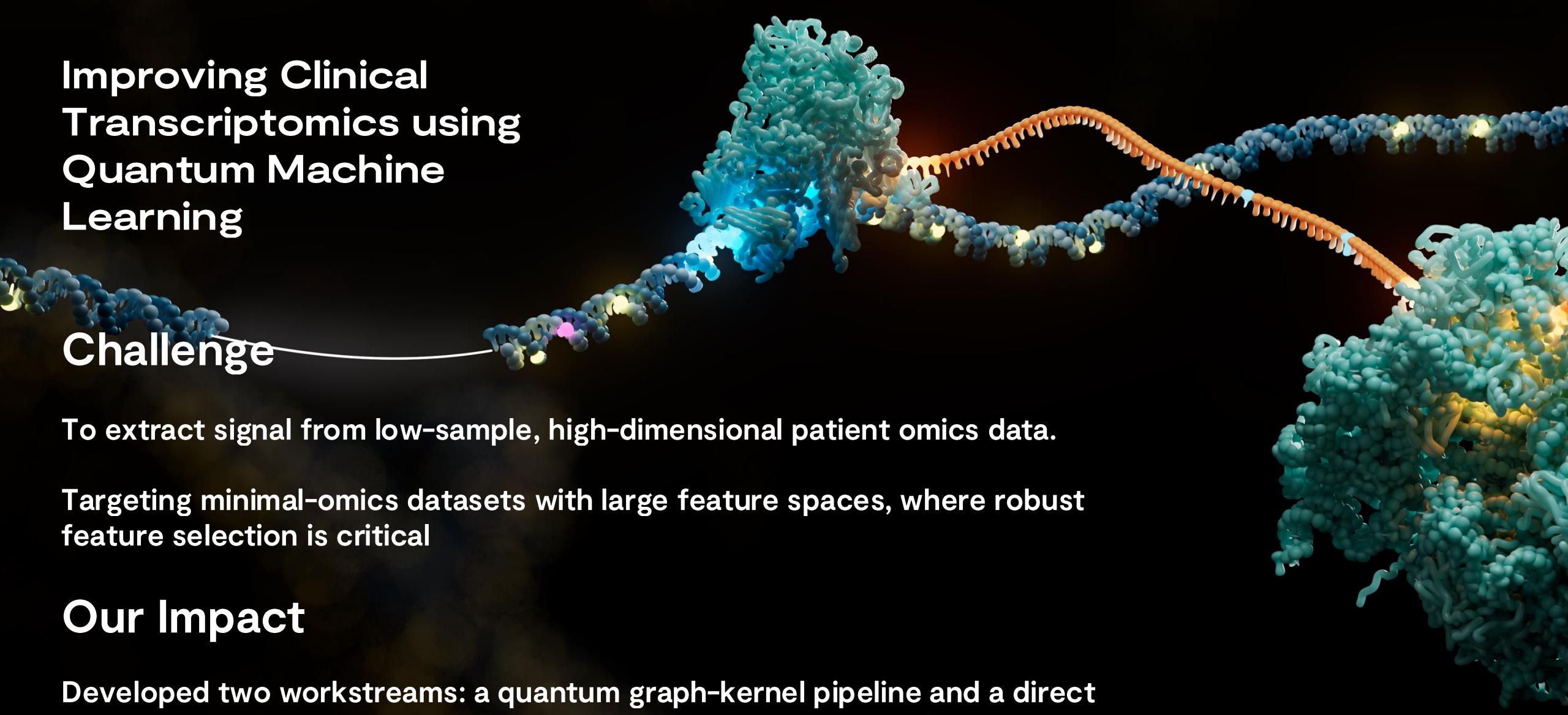
UKRI Science and Technology Facilities Council
Hartree Centre

IBM

NHS
Royal Brompton & Harefield
NHS Foundation Trust

IMPERIAL

Improving Clinical Transcriptomics using Quantum Machine Learning



Challenge

To extract signal from low-sample, high-dimensional patient omics data.

Targeting minimal-omics datasets with large feature spaces, where robust feature selection is critical

Our Impact

Developed two workstreams: a quantum graph-kernel pipeline and a direct quantum vs classical kernel embedding approach

IBM

Cleveland Clinic

UKRI Science and Technology Facilities Council

Hartree Centre

CGA
SIMULATION

Challenge

How to measure quantum resources required to perform Nuclear Magnetic Resonance simulations for practical models of batteries

Our impact

We provided guidance to the quantum resources required to perform NMR simulations for practical models of batteries on future quantum computers.

UKRI Science and Technology Facilities Council

Hartree Centre

QUANTINUUM

Challenge

Can quantum enhanced optimisation can overcome scalability and speed limits of classical solvers in decentralised peer-to-peer energy trading.

Our impact

Defined when quantum approaches outperform classical methods, delivered integration-ready architectures for future P2P energy systems, and provided evidence for the commercial and operational viability of quantum optimisation in future decentralised energy systems.

e·on

IBM

UKRI Science and Technology Facilities Council

Hartree Centre

Challenge

How to adapt quantum simulation code to real world hardware

Our impact

- Support to run the simulation code on IBMQ for their defence customers
- Identify use cases
- Academic Paper

IBM

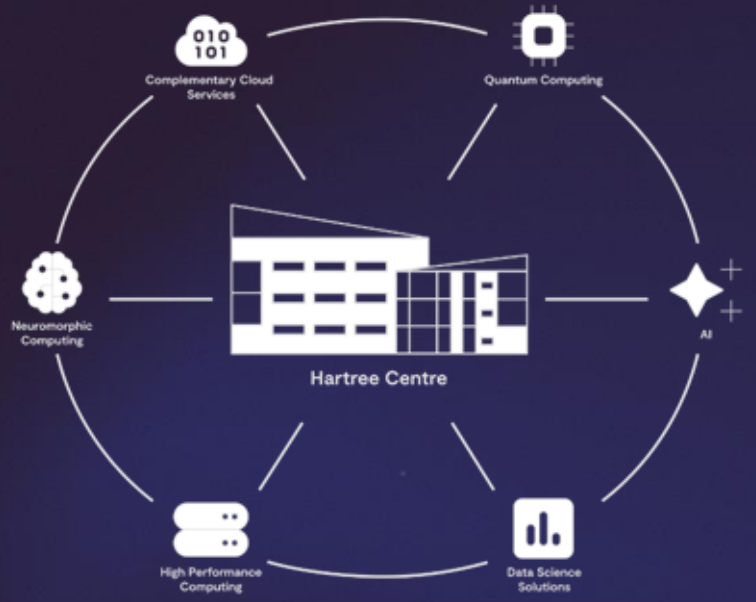
QINETIQ

UKRI Science and Technology Facilities Council

Hartree Centre

Science and Technology Facilities Council
Hartree Centre

Convergence of Technologies



Integrating HPC and QC is a complex

Recognised as a core need to enable the near-term success of quantum computing.

- **Infrastructure** – Bridging fundamentally different hardware architectures
- **Software** – workflow management, resource scheduling and orchestration.
- **Applications** – Adapting and optimizing workflows across quantum and classical domains
- **Ecosystem Development** -Life Sciences, Aerospace and Defence, Transport

Visit our website

hartree@stfc.ac.uk

STFC Hartree Centre

Science and Technology Facilities Council

Hartree Centre

Image credits: STFC Hartree Centre, Adobe Stock