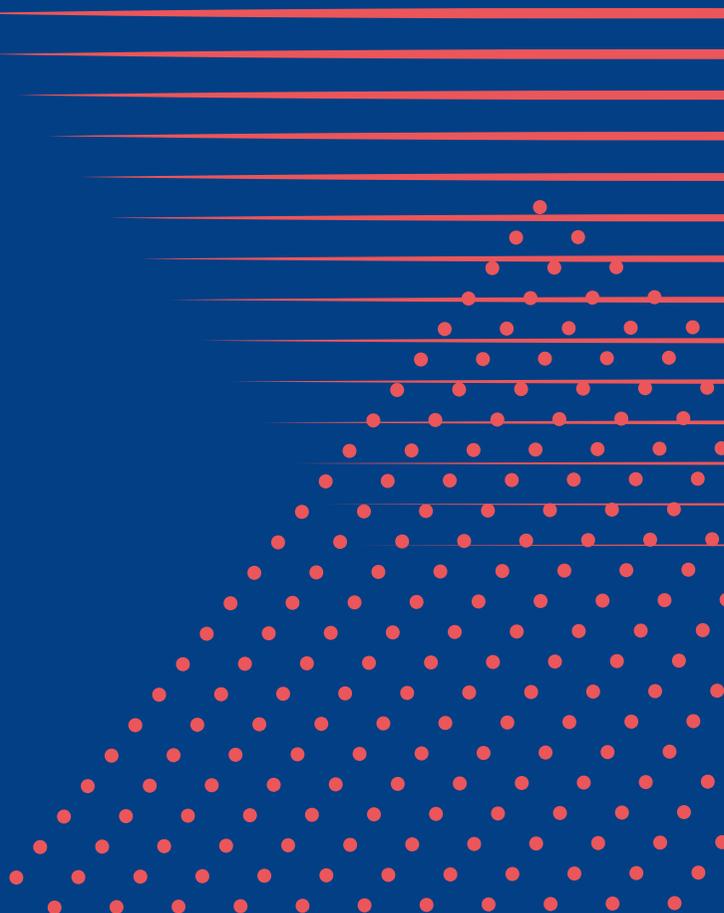# Highlights

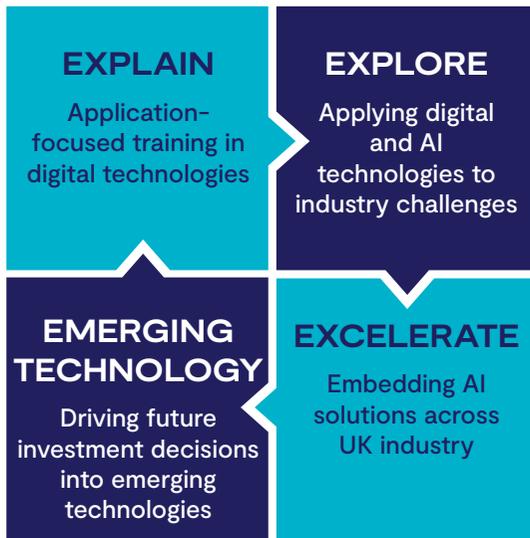## Hartree National Centre for Digital Innovation

May 2023

Highlights

Hartree National Centre for Digital Innovation

We're enabling UK businesses and the public sector to explore and adopt digital technologies including AI and quantum computing for productivity, innovation and economic growth.

The Hartree National Centre for Digital Innovation (HNCDI) is a collaborative programme with IBM Research that offers a supportive environment for organisations to explore the latest digital technologies and skills, develop proofs-of-concept and create roadmaps to apply them to industry and public sector challenges. It is driven by industry requirements and helps organisations with an appetite for change to create innovative, useful solutions, enhance and adapt products and processes, adopt new digital technologies and expand into new markets.

In 2023, the Technopolis Group completed the first evaluation of HNCDI. Here, we summarise the key activities and highlights during the first 18 months of the programme up to December 2022.

EXPLAIN
Application-focused training in digital technologies

EXPLORE
Applying digital and AI technologies to industry challenges

EMERGING TECHNOLOGY
Driving future investment decisions into emerging technologies

EXCELERATE
Embedding AI solutions across UK industry

Four workstreams across the HNCDI programme

Creating an impact through collaboration

HNCDI has expanded the capacity of both the Hartree Centre and IBM and has already seen new types of collaboration with UK industry beginning to emerge with interactions across each of the programme's four workstreams and a pipeline of potential projects and collaborators that builds on lessons learnt in the programme so far.

As of December 2022, the programme has launched 44 R&D projects which have already started producing results with 10 peer reviewed publications published so far and two patent submissions in progress.

10 peer reviewed publications

44 R&D projects launched

EXPLAIN | Application-focused training in digital technologies

Our training is application focused, designed to enable individuals, businesses and public sector organisations to take advantage of digital technologies like supercomputing, data science, AI, full stack, cloud and quantum computing to enhance processes within your organisation and provide the skills needed to thrive in a digital economy.

NSG Pilkington embrace data science

NSG Pilkington manufactures and processes glass for the architectural and automotive sectors. Collaborating with the Hartree Centre on two materials discovery projects inspired a company-wide recognition of potential data science applications. NSG piloted a programme to train their staff in data science through the HNCDI EXPLAIN training programme, recognising the Hartree Centre as a reputable and trusted source working at the cutting edge of digital technologies.

The company was drawn to the flexible course delivery and range of experience levels, ensuring consistency in approach and terminology. From materials science to legal teams, NSG staff registered for 61 courses from beginner to advanced level and reported improved confidence in framing and communicating their requirements to data science experts. Others suggested they felt more ready to tackle internal data science challenges and have recommended the training to new data science recruits demonstrating the usefulness and wide application areas of the range of courses on offer.

544 attended training courses

239 organisations registered

EXPLORE | Applying digital and AI technologies to industry challenges

We're solving industry challenges when there isn't an existing off-the-shelf solution but there is evidence it can be solved and a business value and motivation to solve it. Our team use their expertise to develop new capability demonstrators that are designed to solve practical challenges for your industry. By cultivating and maintaining strong connections to the UK's fundamental research base, we develop tools and techniques that improve societal and economic outcomes.
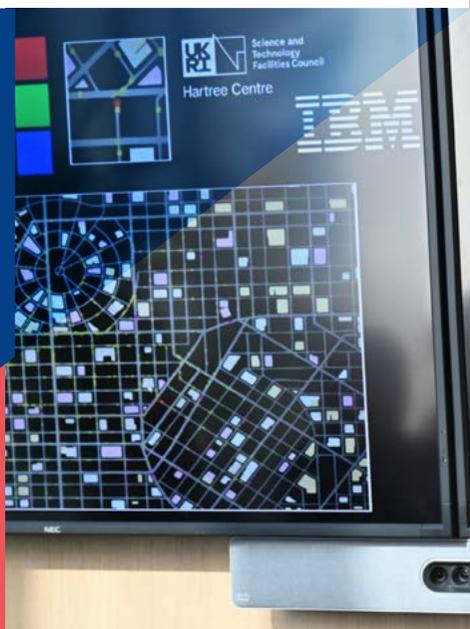
Using AI to map the risk of flooding

Mapping the risk of climate events requires the analysis of massive datasets, usually done through a time-consuming, semi-manual process. Through HNCDI EXPLORE, we developed a machine learning algorithm to identify past and current flood events using satellite data. Our team trained the algorithm using suitable open-access ground-truth data, verifying this capability against a set of known flood events. Applying AI accelerates the process of identifying and labelling flood event data, which is fed into a suite of related modules all hosted on a cloud platform called the Geospatial Discovery Network (GeoDN). This platform can map climate events and improve the resilience of UK infrastructure, enhancing our capability to address damage and prepare crisis responses across multiple climate applications.

EXCELERATE | Embedding digital solutions across UK industry

We're using applied research and innovation to turn good ideas into industry-ready solutions that address business challenges. By collaborating with our industry partners, we are lowering the barriers to innovation, creating enhanced products and services and generating long-term societal and economic impact. Our HNCDI collaborators report increased confidence in technological solutions for digital transformation and innovation.
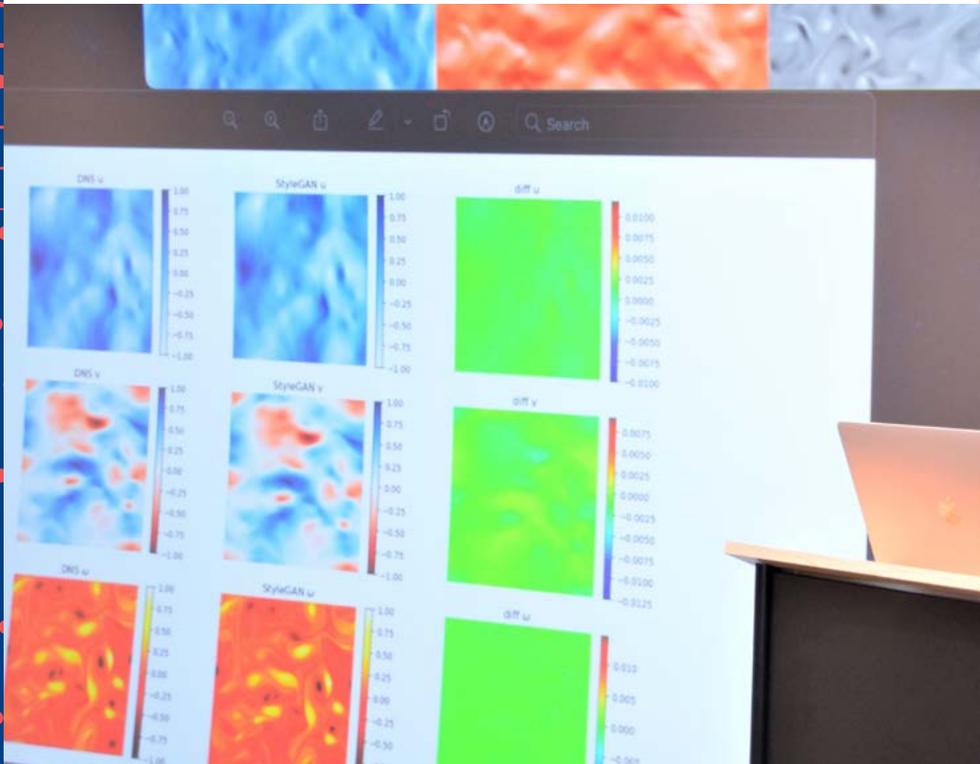
## AI powered precision medicine for Inflammatory Bowel Disease (IBD)

Through HNCDI EXCELERATE, Biotech company Reprocell accelerated the development of machine learning algorithms used in precision medicine strategies by working with the Hartree Centre and IBM on an AI-powered platform capable of simplifying complicated datasets. Through this collaboration, pharmaceutical companies can streamline drug development processes and identify more effective treatment for those suffering from Inflammatory Bowel Disease (IBD) quickly and cost-effectively with the potential to expand out into cancer therapies, transforming drug development and clinical trial timescales and efficiencies. Together we're making a step towards increasing the scope and capacity of precision medicine in a commercial environment.

EMERGING TECHNOLOGY |
Driving future investment decisions into emerging technologies like quantum computing

We are looking to the future of computing in the UK, helping to identify the areas where emerging digital technologies like quantum computing might offer the most competitive advantage. By looking at the intersection of existing classic high performance computing applications and exploring quantum technologies, we want to enable effective investment decisions to make your business or organisation more resilient and unlock new possibilities.
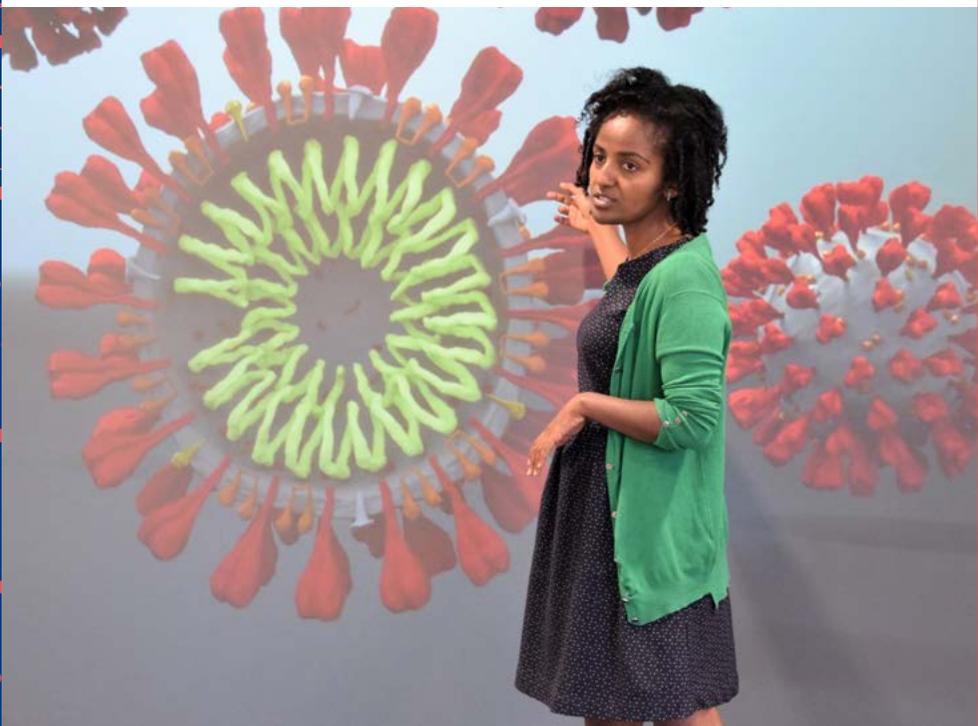
## Quantum Machine Learning strategies for accelerated drug discovery

In the HNCDI EMERGING TECHNOLOGY workstream, the Hartree Centre and IBM investigated the potential of quantum computing to accelerate the drug discovery process and reduce costs through Ligand-Based Virtual Screening, a computational technique that screens digital databases of molecules to identify structures most likely to bind to a drug target. The project demonstrated that the Quantum Support Vector Classifier often performed better than the equivalent classical HPC algorithm and sometimes greatly outperformed the deep learning methodologies that are currently state of the art in drug discovery.

Training traditional machine learning algorithms can be prohibitively resource intensive, so quantum-enabled machine learning offered a potential advantage by supporting calculations at exponentially higher-orders of complexity to increase efficiency and accuracy. In February 2023, the team published a paper on the results and are scoping potential follow-on projects with UK pharmaceutical companies. This knowledge discovery saw a new concept and approach – integrating and applying quantum computing to drug discovery and life sciences.

SME Engagement Hubs

In Summer 2023, the Hartree Centre will launch a network of three HNCDI Hubs across the UK. Each hub will be established with regional partner organisations and each will have a purpose of engaging their local or sectoral networks to increase the adoption of digital technologies. They will have a remit to upskill SMEs in their area by delivering short collaborative projects and training to facilitate journeys in digitalisation for businesses regionally, expanding the reach of the Hartree Centre.
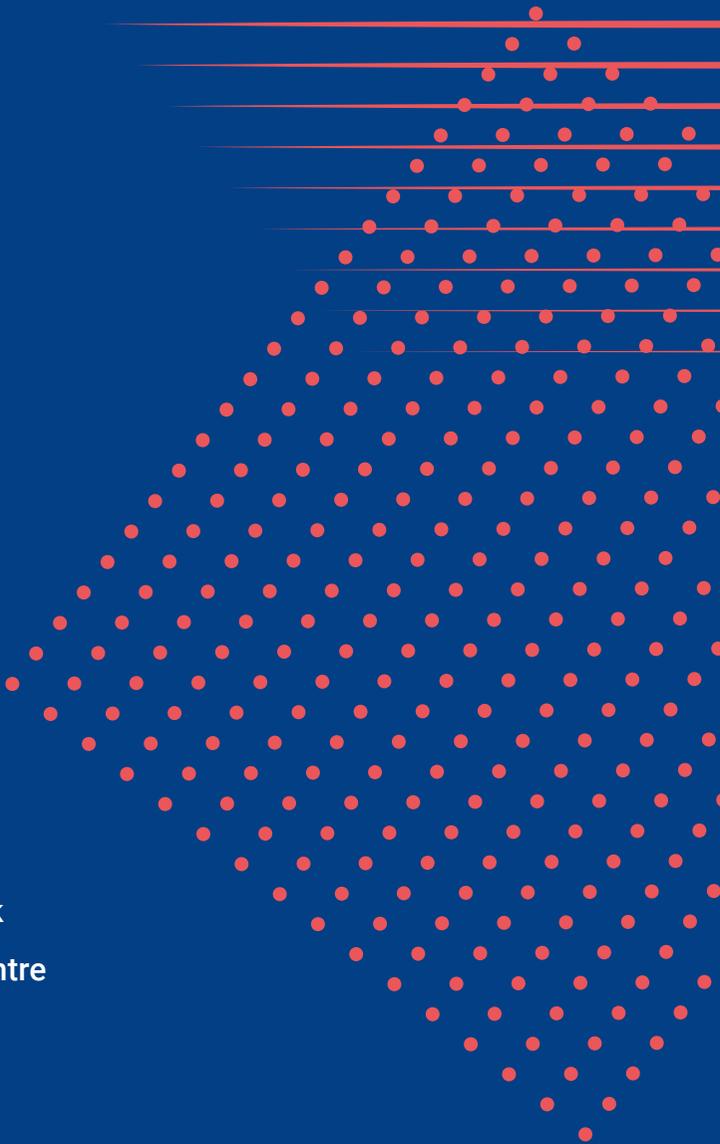
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