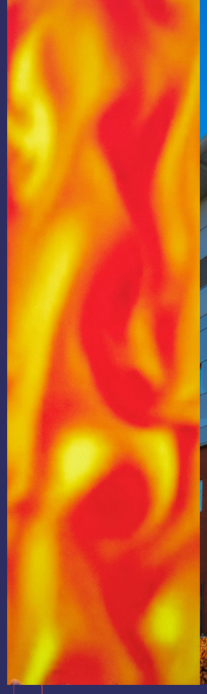


Science and Technology Facilities Council
Hartree Centre

IBM

HARTREE NATIONAL CENTRE FOR DIGITAL INNOVATION

PROGRESS REPORT

2025

Science and Technology Facilities Council

Hartree Centre

Hartree National Centre for Digital Innovation Progress Report

For the period January – December 2024

Lizahn van Gend, Adebisi Adewusi, Charlotte Glass, Neil Brown

March 2025

Table of Contents

Executive Summary 3
1. Introduction 5
This report and methodology 6
2. HNCDI Programme Progress Overview 7
3. Collaborative R&D Projects – Emerge, Explore, Excelerate 9
Emerging Technology 10
Explore 13
Excelerate 16
4. Engagement – SME Hubs 18
5. Training – Explain 23
6. E-infrastructure – Cloud, On-premise Cloud and the Supercomputing Centre 24
Appendix – Interviews 26

This report was prepared by Technopolis, an independent policy and evaluation consultancy, on behalf of the Hartree Centre.

Executive Summary

The Hartree National Centre for Digital Innovation (HNCDI) programme has been running for three and a half years and is making good progress towards achieving its targets. With one and a half years remaining, HNCDI has established itself at the forefront of innovation in converged digital technologies for industry challenges.

The programme aligns closely with the STFC Hartree Centre's overarching strategy to champion the adoption of innovative digital technologies. Through its initiatives and collaboration with IBM, HNCDI has significantly advanced the Centre's expertise in critical and emerging areas. Delivered across six core workstreams, and supported by a central programme management team, HNCDI supports collaborative projects (through the Explore, Excelerate, and Emerging Technology workstreams), delivers training and SME engagement (through the Explain workstream and three regional SME Engagement Hubs) alongside a range of e-infrastructures hosted by the Hartree Centre and IBM.

The technology landscape has seen major shifts in recent years, including the increased application of Artificial Intelligence techniques, development of Quantum Computing (QC) capabilities and public cloud storage. In this context, it can be challenging to avoid hype cycles and pin down the real forefront of technology, yet the programme has remained relevant and a key source of expertise throughout.

This document presents a third progress report for HNCDI, delivered as part of a wider programme of monitoring and evaluation support provided by Technopolis. It outlines the progress, successes and challenges in driving forward HNCDI between January and December of 2024.

Highlights:

- The programme's rapid application of lessons learned during its first half has enabled the industry adoption-focused Excelerate workstream to establish a strong pipeline of projects. There is now a healthy flow of projects from Explore into Excelerate, supported by the relationships built through both workstreams' involvement in setting up sector-themed project calls.
- The HNCDI Emerging Technology team has established itself as a global leader in quantum computing for industry, exceeding its original project targets and fostering strong collaborations. It plays a major role in the QC sector by maintaining and developing IBM's Qiskit Machine Learning, an open-source tool for interfacing with Quantum Neural Networks and other machine learning methodologies. Recognised as an IBM Quantum Innovation Centre, the team manages unprecedented access to premium quantum machines. HNCDI has therefore become a sought-after partner in a resource-limited field, leading to high-profile collaborations and substantial partner commitments. The team actively shares its research through global conferences, industry events, and several IBM-led global working groups (e.g., optimisation problems, healthcare and life sciences, and high energy physics). With its scientific outputs and strategic capabilities, the programme is also well-placed to support the UK's National Quantum Strategy.
- The industry relationships and technologies developed within Explore have been consolidated into a tangible asset for the wider programme. Each of its key technology areas has seen solutions taken forward and expanded into the Excelerate workstream, having attracted the interest of external organisations to take these forward into real-world applications.
- The three SME Hubs, based in Cardiff, the North East of England and Northern Ireland, continue to extend the geographic reach of programme. Each Hub leverages its own networks and resources to reach and assist SMEs in their region with the adoption of digital technologies; while also creating awareness of resources available from the wider programme (such as Explain training courses). The Hubs have engaged with over 200 SMEs in their local areas so far.
- Across the collaborative R&D (CR&D) workstreams: Emerging Technology, Explore and Excelerate, 123 projects have been launched (as of December 2024), while 60 have been successfully completed. In parallel, these workstreams have engaged 59 unique partner organisations and secured more than £3m of in-kind contributions. Projects have started to produce codified knowledge, demonstrated in 43 peer-reviewed publications, and several patent submissions are also in progress.

- Over 2,300 individuals have attended training courses hosted on Explain's dedicated, free-to-access online learning platform.
- The Hartree Centre's Supercomputing Centre (SCC) building is complete. It now awaits the internal mechanical infrastructure and the high-performance computer itself, with installation expected in May 2025. Once done, the SCC will be handed over to STFC to configure and integrate and is intended to be fully operational by the end of 2025.

1. Introduction

The Hartree National Centre for Digital Innovation (HNCDI) was launched in June 2021 to drive the development and adoption of emerging digital technologies in the UK, including High-Performance Computing (HPC), Artificial Intelligence (AI) and Quantum Computing (QC). Based on a five-year collaborative agreement between the STFC Hartree Centre and IBM, it supports UK businesses and public sector organisations, large and small, in their journey to develop innovative solutions to common industry challenges. The aim of the programme is to provide the support needed to enable UK organisations to understand the potential of digital technologies like AI and QC for their business and to accelerate the adoption of advanced digital technologies.

Over the past three and a half years, the HNCDI programme has established a unique position in the UK's R&I landscape and is a key contributor to addressing and realising national strategies and priorities. In particular, **Invest 2035: the UK's modern industrial strategy** (2024), recognises digital and technologies as a growth-driving sector, and identifies opportunities for AI and quantum technologies across multiple sectors like professional business services, life sciences and defence. The government has also published its intentions to drive the adoption of AI in the civil services sector in the **AI Opportunities Action Plan** (2025). HNCDI is a key contributor to addressing these challenges, providing training and access to the computation facilities of both the Hartree Centre and IBM Research, as well as access to specialist knowledge and expertise.

The HNCDI programme employs a multi-layered approach to supporting R&D and the adoption of AI and QC technologies facilitated by HPC. To deliver against its aim, the programme is comprised of five main workstreams of activity to address four key stages of digital adoption:

- **Explain** – the provision of accessible and application focused training courses that span a range of digital economy topics, such as AI, machine learning, reinforcement learning, high performance computing and quantum computing. Courses are delivered in a variety of formats, from self-paced e-learning to live sessions and workshops.
- **Explore** – proof-of-concept developments that target the frontier of AI and digital technologies. In collaboration with potential industry users and supply chains, projects identify real-world challenges and develop digital solutions and minimum viable products with high potential value to industry.
- **Excelerate** – these collaborative projects aim to take a business challenge and develop solutions ready for adoption and integration into a specific industry partner.
- **Emerging Technology** – combining established high-performance computing techniques with emerging technologies like quantum computing, this workstream aims to improve the understanding of their potential for industry application.
- **SME engagement** – The HNCDI programme has established three SME Engagement hubs across the UK to engage with the wider SME community and provide an initial entry point to launch their digitalisation journey. Delivered in collaboration with three delivery partners, the Hubs deliver short projects/interventions and engagement.

Two further workstreams of activity underpin these workstreams:

- **E-infrastructure** – enabling the procurement and construction of a more efficient supercomputing centre at STFC's Daresbury Laboratory, the provision of a new supercomputer that has AI-capability. It will run containerised workflows as well as 4 GPUs on every node. This work is complemented by the procurement, and provision of a hybrid cloud platform.
- **Programme management** – supporting programme delivery through project management, programme monitoring, evaluation and communications activities, and cross-programme activities, including recruitment and running seminars and workshops outside workstreams.

This report and methodology

This document is the third and final annual progress report for the HCNDI programme and presents developments and emerging results for the period January-December 2024. The methodology used to prepare this report has been aligned with the objectives set out in the Evaluation Framework Report (May 2022) and combines:

- **Interviews** with 10 members of the HNCDI programme delivery and senior management teams. These interviews focused on each of the key programme workstreams – Explain, Explore, Emerging Technologies, Excelerate, E-infrastructure, and each of the three SME Hubs. The list of interviewees is presented in the Appendix – Interviewees.
- **Desk research and review of programme documentation**, including review and analysis of HNCDI KPIs, project management documents (PMDs) and project summaries, board presentations, and survey feedback.
- **Regular conversations with the Impact Evidence and Evaluation Manager –** Fortnightly online meetings to discuss programme progress.

The remainder of this report is structured as follows:

- **Section 2** presents an **overview** of the HNCDI programme's progress and emerging benefits.
- **Section 3** presents the progress of the programme's collaborative R&D (CR&D) workstreams – **Emerging Technology, Explore** and **Excelerate** – including key outputs and outcomes of the programme to date and case studies highlighting emerging impacts emerging from projects.
- **Section 4** presents the progress of HNCDI **SME Engagement Hubs**, their implementation and emerging benefits.
- **Section 5** presents the HNCDI's training activities through the **Explain** workstream.
- **Section 6** presents the progress and benefits emerging from the HNCDI's **e-infrastructure**.
- **The Appendix** contains a list of stakeholders interviewed for this report.

2. HNCDI Programme Progress Overview

HNCDI translates High Performance Computing (HPC), Artificial Intelligence (AI) and emerging technologies such as Quantum Computing (QC) into scalable tools and techniques for adoption by UK businesses and the public sector. It provides support to enable UK organisations to better understand the potential of digital technologies and future computing initiatives for their business, accelerating the adoption rate and benefits realisation for UK industry.

The Hartree Centre and IBM collaboration epitomises the integration of public and private research excellence. It has created tangible value for partners by providing access to a wide range of expertise and resources like quantum computers and HPC. HNCDI stands out as the only programme offering converged digital technology solutions for industry, tailoring and building its approaches — QC, AI, or other technologies — to the unique socio-economic challenges at hand. This approach ensures maximum impact and problem-solving efficacy for its partners.

As of December 2024, the programme is three and a half years into its five-year funding period and has hit its stride by most measures. HNCDI has reached a critical mass of internal capability in cutting-edge digital technologies, and its reputation and relationships with external organisations enables the programme to attract high-quality projects. The Hartree Centre remains the UK's only supercomputing centre dedicated to industry and the HNCDI programme continues to adapt in response to the rapidly evolving digital technologies landscape. It maintains expertise in key areas like quantum computing (QC), machine learning (ML) and large language models (LLM) and the combination and convergence of these technologies to provide the optimal solution for project partners, is an emerging benefit.

The programme has maintained a flexible and responsive approach to capacity and resource planning, ensuring both are sufficient to deliver against its targets by the end of the current programme in 2026. From recruitment through to delivery, the team's mix of skills is continuously adapted to reflect the needs of the programme and projects. The internal capacity of the team has also been complemented by the increased interest from industry partners to embed their staff within the HNCDI programme to enhance capacity building and exchange knowledge within their organisations.

Compute requirements have shifted significantly since the programme's design. HNCDI has stayed on top of this through the procurement of public cloud services and cloud-access to IBM's quantum computer. The adoption of public cloud providers has made it possible to integrate a rapidly growing technology – Large Language Models – which was not anticipated at the start of the programme. This highlights HNCDI's ability to adapt to the evolving digital landscape.

The programme has undertaken a breadth of communications and engagement activities in the broader national AI landscape, including high-profile events such as the UK Government AI Summit, the Liverpool City Region AI Summit, and the Alan Turing Institute's AIUK conference. HNCDI showcases its work at these events through staff participation, case studies, and fringe events, securing valuable leads and demonstrating its contributions to the digital innovation ecosystem.

The Explore and Excelerate workstreams collaborate on open calls for projects dedicated to a specific sector. The sector calls have yielded a handful of projects, though the calls' key benefits to the programme lie elsewhere. With the help of sector bodies like NAFEMS[1] (for simulation) and the APC[2] (for automotive), new partnerships have been established and offers have been tailored to industry-specific needs, increasing the programme's attractiveness to industry.

Implementing lessons learned in project administration, the Project Management team now operates with a high degree of independence for functions like costing, setting up and closing projects, and in

[1] National Agency for Finite Element Methods and Standards, https://www.nafems.org/2018/uk/

[2] https://www.apcuk.co.uk/

facilitating resources for project delivery, enabling project teams to maximise their productivity and accelerating the flow of project pipelines.

As the programme has gained momentum, benefits to society are being realised through four key mechanisms:

- **Adoption of digital technologies** e.g., in the Excelerate and Explore workstreams, where solutions developed for partners like REPROCELL, Royal Haskoning DHV and Dark Matter Labs are entering their evaluation license period – a set time over which project partners have free access to the technology developed in order to integrate it with their operations and suggest modifications.
- **Development of digital assets with high relevance to industry** e.g., in Explore, working closely with sector bodies and industry partners to understand end-user needs and develop highly applicable assets. Asset reuse in the CR&D workstreams is at its highest level since the launch of the programme, especially as continuous engagement and follow-on projects deepen relationships with partners like the UKAEA (to solve fusion problems), the Cleveland Clinic in London (for healthcare applications), and AstraZeneca (for drug discovery).
- **Development and publication of new knowledge** e.g., in Emerging Technology, dozens of publications have emerged in the area of Quantum Computing methods. The HNCDI team are leveraging their exceptional access to physical quantum computers to conduct research and build methods in a way that simulated quantum computing environments cannot offer.
- **Upskilling for adoption** e.g., in the Explain workstream, in which project partners are offered courses that are relevant to project solutions, to build internal capability and increase the likelihood of successful integration with the organisation once the project is done.

The effectiveness of these mechanisms is driven in part by close collaboration between the programme workstreams. For example, Explore and Excelerate have progressively combined their project identification and initiation processes to enable a strong flow of projects from the research phase through to adoption, as was intended at the start of the programme. Emerging Technology and Explore are also collaborating on hybrid-technology applications by exploring the use of AI to optimise quantum circuits for materials simulation on quantum computers.

The programme's progress is confirmed by positive feedback and a full green rating from DSIT after their Gateway 4 review over the summer of 2024.

Overall, HNCDI is well-positioned to achieve its targets, and focus is shifting toward delivering a strong conclusion to the current programme. Efforts are also underway to secure continuity and maintain stakeholder buy-in for a potential follow-on initiative, HNCDI phase 2, which would build on existing partnerships and project pipelines.

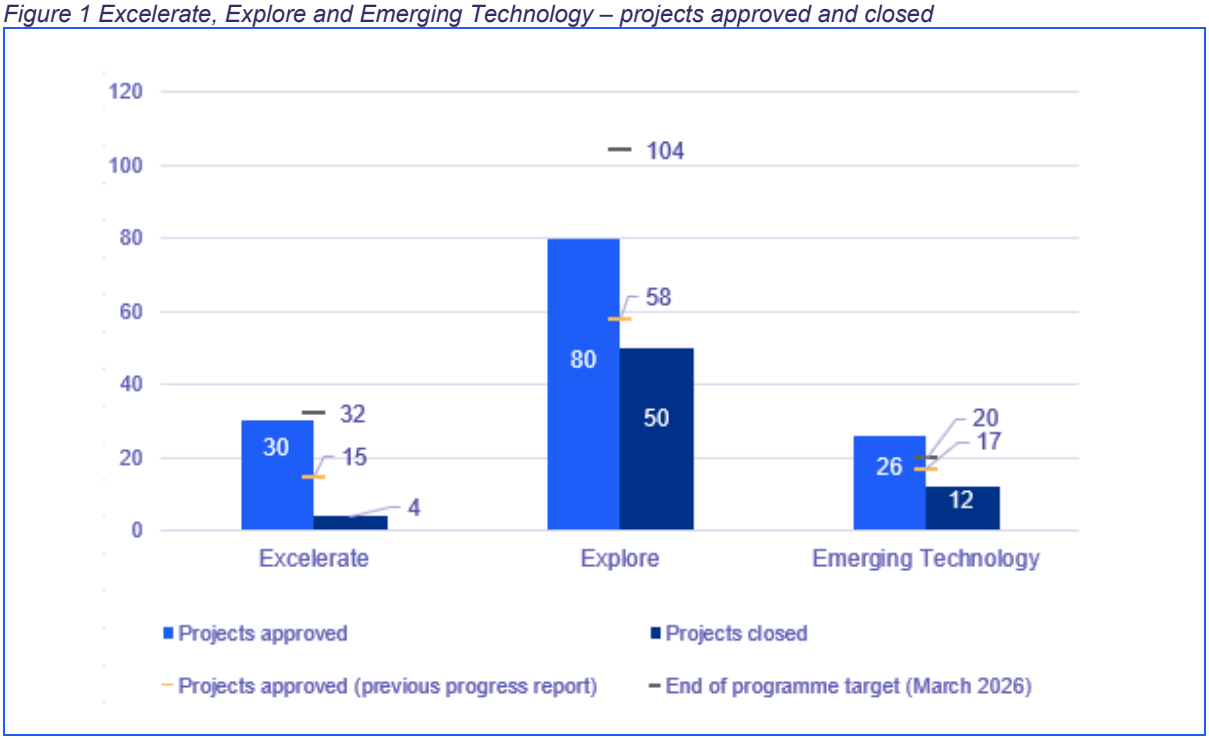
3. Collaborative R&D Projects – Emerging Technology, Explore, Excelerate

Emerging Technology, Explore and Excelerate are the three core R&D (CR&D) workstreams for the HNCDI programme. Each focuses on technologies at different stages of their development.

Across these workstreams, the HNCDI programme has **approved 136 projects**, an increase of 46 since the last progress report (December 2023) and 87% of the programme target of 156 projects. 60 of the 136 approved projects have closed successfully, with a further 57 ongoing. As of January 2025, five projects await kick-off.

The figure below suggests that all three CR&D workstreams will **reach or exceed their target number of projects** while emphasising the need to focus on project closure – especially in Excelerate, which has approved 81% of its target projects. This has been a positive shift since the previous reporting period, in which Excelerate was struggling to approve and start projects and falling short of its targets. At HNCDI's midpoint, the workstream had yet to approve half of its target project approvals, but now only six projects remain to reach the programme's goal. Emerging Technology has surpassed its objectives in terms of projects approved by 30% and is leveraging efficiency gains and partner contributions to continue working without additional budget. Explore, the largest of the workstreams with respect to the number of projects, has approved 77% of its target and is on track to meet its objectives by 2026.

Figure 1 Excelerate, Explore and Emerging Technology – projects approved and closed



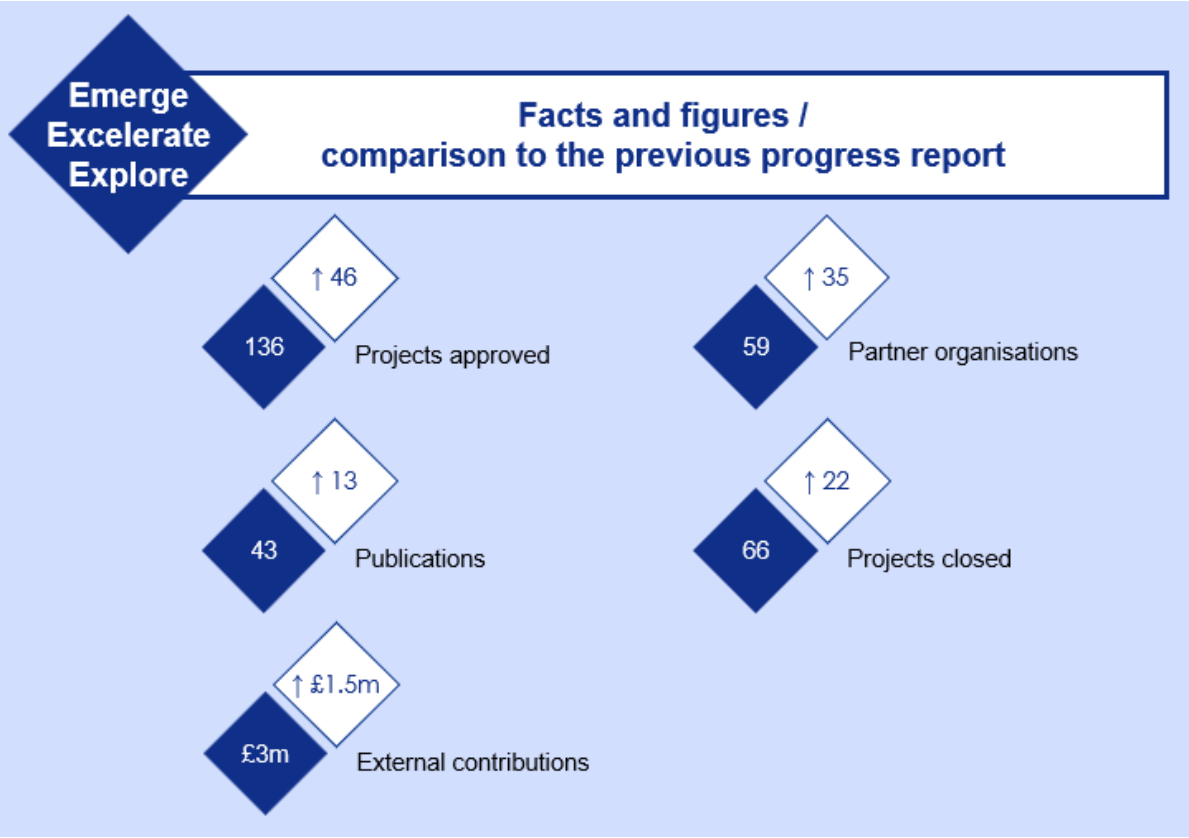
Source: HNCDI monitoring data.

The three workstreams have so far engaged **59 partner organisations** from a variety of sectors and spanning a range of different sizes. The CR&D workstreams have also secured over **£3m**[3] **in in-kind contributions** from these partner organisations – an increase of £1.5m since the previous reporting

[3] Estimate based on staff time for closed projects, as well as estimations of the value of any software, code or data contributions to those projects. Note that the value from the 18-month progress constituted only staff time.

period. This continued investment and support demonstrates the value of collaborative R&D carried out through HNCDI.

The programme has continued to produce new codified knowledge – HNCDI researchers have created an additional 13 peer-reviewed publications since the last report, adding up to a **total of 43 publications** overall. Furthermore, the utility of programme software is being demonstrated through redeployment in other parts of HNCDI.



Source : HNCDI monitoring data

Emerging Technology

The HNCDI Emerging Technology team has made strides in advancing the field of quantum computing, establishing itself as a global leader in this rapidly evolving field. The workstream attracts continuous interest and demand for collaboration from industry and has established relationships with organisations like IBM Quantum and the NQCC.

The workstream has exceeded its original target of 20 projects, now managing 26 and expecting to complete more than 30 before the programme concludes. More than half of these projects involve collaboration with external partners, demonstrating the interest from industry in quantum computing. High-profile collaborations, such as with AstraZeneca, have resulted in multiple projects and substantial partner commitments, including in-kind contributions that have extended the workstream's capacity to deliver projects beyond original target numbers. Another key enabling factor is the efficiency gained by the team since the programme's launch; their considerable experience with quantum solutions has cut down development and testing to a fraction of the time.

The team actively disseminates their research, for example, by offering workshops at IEEE Quantum Week and tutorials at global conferences like the European Supercomputing Conference. They also

participate in IBM-hosted healthcare events that engage with drug discovery companies, clinicians, and government stakeholders, and they contribute to courses offered through Explain. The team has participated in IBM's global working group on quantum optimisation[4]. The group focuses on finding quantum computing methods of optimisation that have a clear advantage over classical computing methods, and it consists of over 40 organisations. This, in turn, has yielded new collaborations and publications for the programme.

Emerging Technology also drives access to and adoption of quantum technologies in other ways. For example, the workstream maintains IBM's Qiskit Machine Learning package, an open-source platform for organisations interfacing with Quantum Neural Networks (QNN). The team is responsible for developing and maintaining the package's compliance with IBM's evolving quantum devices. So far, Qiskit Machine Learning has been downloaded over 550,000 times and is slated for a major update (Version 1.0) in 2025. Emerging Technology has also increased the likelihood of adoption with QC by focusing on projects with industrial applications, such as simulating energy dissipation in materials. These projects draw on classical AI to optimise the model's quantum circuits and will address real-world challenges like the development of molecules to harvest light used by plants for photosynthesis.

In recognition of their work on HNCDI, the Hartree Centre has been recognised by IBM as a Quantum Innovation Centre, which grants the Emerging. Technology team the authority to delegate access to IBM's premium quantum computing machines for HNCDI projects and beyond. This resource is fully utilised, with 28 people across 17 projects, using 9 of IBM's machines. It is noteworthy that this is an unprecedented level of access, demonstrating that the Hartree Centre is a highly sought-after partner for IBM, in a field where the scarcity of quantum machines means that scientific work is often done in a simulated quantum environment. At the Hartree Centre, the industry validation of quantum applications takes this work further. The programme's relationship with the NQCC also facilitates the possibility of additional quantum computer access if needed, reinforcing the value of public-public partnerships through UKRI.

The scientific outputs of Emerging Technology are a powerful means of attracting potential industry partners and adoption projects. The team has produced several peer-reviewed publications on quantum computing methods, which have gained the interest of experts in the field.

The expertise and resources available within the Emerging Technology workstream mean that the programme is well-placed to provide strategic advice to government and policymakers, especially in the context of the **National Quantum Strategy (2023)**.[5]

[4] https://www.ibm.com/quantum/blog/quantum-working-groups

[5] https://assets.publishing.service.gov.uk/media/6411a602e90e0776996a4ade/national_quantum_strategy.pdf

Explore

Case study
Monitoring soil health with AI

Predicting soil carbon content through a combination of microbial and environmental data, Rothamsted Research and the Hartree Centre are using AI to create new insights into how ecosystems respond to environmental stressors and develop strategies to mitigate the effects of climate change.

The Challenge

Soil health impacts food security and the climate through its ability to capture carbon, so it is crucial for us to know how it works. However, soils are the most complex biological systems on earth, and understanding how they respond to different environmental factors means analysing vast amounts of data. For this reason, Rothamsted Research collaborated with the Hartree Centre through the HNCDI programme to develop an AI framework that uses metagenomics data (soil microbiome data), soil composition data, and climate data to generate novel insights into soil carbon capture.

The Approach

The Hartree Centre combined their multi-omics and geo-spatial AI-based assets developed in earlier HNCDI projects, while Rothamsted Research ensured alignment of the project's capabilities with the needs of industry. The resulting framework predicts soil carbon content in a process that automates workflow and database construction, making it easy for stakeholders who are less familiar with the project to perform their own analyses if granted access. The framework is not yet capable of analysing data and generating insights at the national level (meaning that the simulations cannot yet operate at that scale) due to the volume of information being processed. However, future iterations of the project aim to resolve this by deploying more modular as well as cloud-based solutions that can overcome compute-time limitations.

The Benefits

The project has enabled acceleration of Rothamsted's bioinformatics pipelines; what would have taken them months to do independently now takes a day using the framework developed with the Hartree Centre. The project has already led to a discovery concerning a particular microbe which may have a pivotal role in soil carbon capture, and the collaboration expects to publish its findings soon. The team's work gained attention from major research institutes which have expressed interest in collaborating on future projects. The framework is also drawing interest from agritech SMEs hoping to use it to improve the fertility of their soil. Furthermore, the framework's versatility opens it up to diverse applications such as monitoring diseases or ocean wastewater levels, and for drug discovery.

Explore

The Explore workstream is realising the benefits of foundations laid in the programme's early years. Explore was designed to pick up early-stage theories and methods in digital technologies and then prove their workability and potential value through a proof of concept (POC). Explore has consolidated the capabilities and relationships with external partners developed in the first years of the programme and is now leveraging these to work directly with organisations to develop highly relevant POCs.

Since the programme was launched, Explore has been developing software assets into themes; clusters of methods and tools that are grouped according to commonality. Whereas early development was somewhat ad-hoc and based on the projects available, the grouping of technology assets built enough momentum to attract and sustain targeted projects, enabling the Explore team to offer consolidated solutions that draw from and build on the success of numerous prior projects. Explore has so far developed three key technology application areas:

- **Materials**: a simulation platform that uses data on known materials' properties to predict the properties of simulated materials. Using ML, the platform can automate the materials discovery process, from simulation of materials through to identification of potential candidates with a target set of properties (such as those needed for a good semiconductor, battery or solar panel).
- **Life sciences, Health and Wellbeing:** a series of solutions utilising multiomics data that uses large datasets of genetic information and combines this with other information. This includes the prevalence of disease in human or animal tissue, or carbon content in soil, to support applications in, for example personalised medicine and environmental sciences (see the case study with Rothamsted Research above).
- **Nuclear, Energy and the Environment**: a platform that combines environmental datasets, like different kinds of satellite images with geolocation data. When integrated with AI, the platform can map climate change weather events such as flooding and predict the potential impact of these events. It can also integrate these insights with other functions and systems, such as investment or disaster warning.

The capabilities developed within Explore are not limited to these three themes, and embedded into the programme is regular innovation to build new tools with highly generalisable capabilities. In one example, a Variational Exploration Model (VEM) that was developed for application with Riskaware, an incident modelling software company, could also be applied to any sector or situation where the outcome of a process is sensitive to many variables.

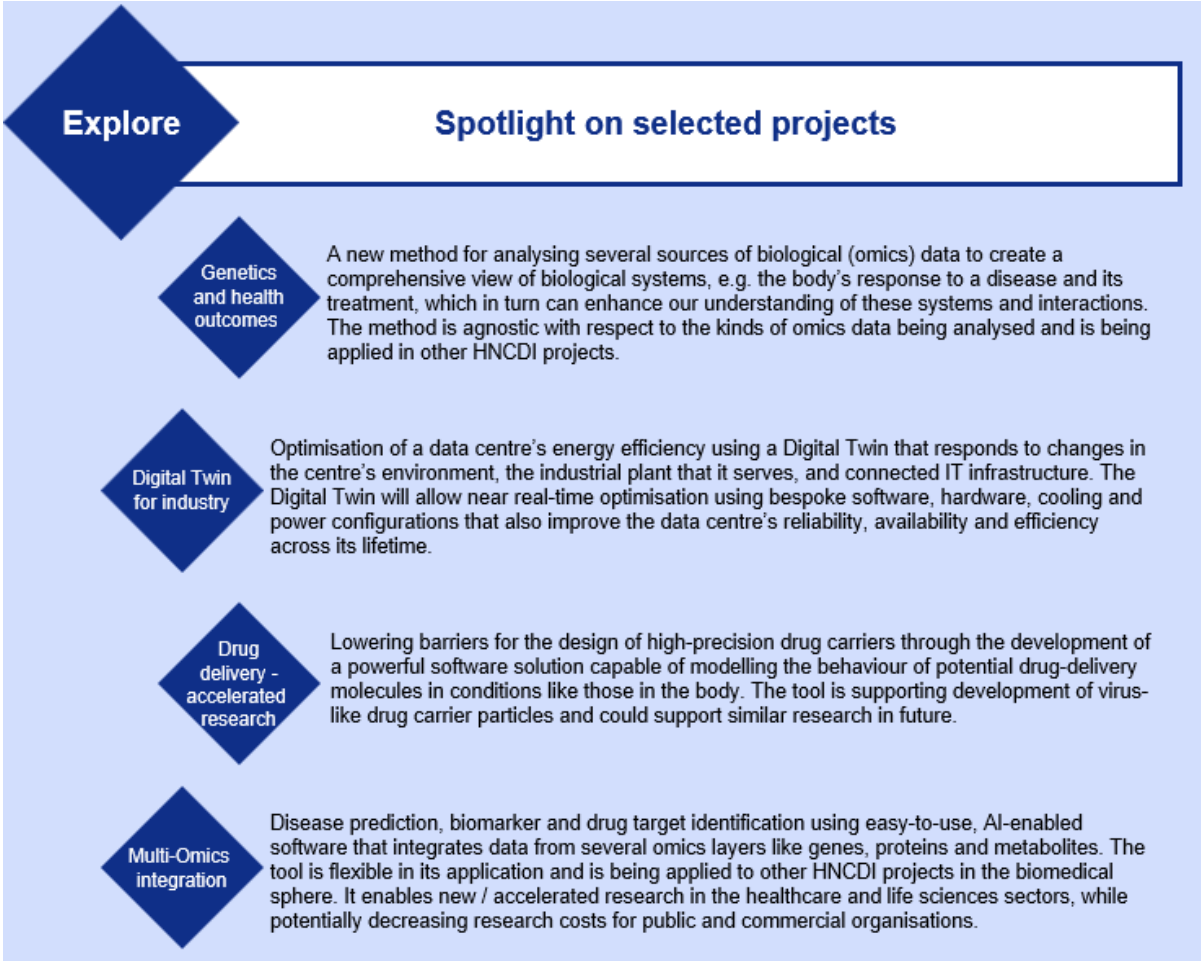
Alongside the Excelerate team, Explore initiated a series of sector-specific calls for proposals e.g., automotive or engineering simulation. These sector calls have been used to identify early-stage technologies with applications relevant to industry and each one has been developed in close collaboration with an expert sector body such as NAFEMS for simulation, or the APC for automotive.[6] The key strength of the sector calls is not the resulting projects but the collaboration with this sector partner. These relationships enable a strategic networking approach that extends beyond the confines of the sector call, and toward individual organisations of interest. The calls have also been excellent for getting an appreciation of sectors' practical needs, which is critical for the relevance of Explore projects.

The Explore team has been working closely with Excelerate to resolve project pipeline concerns that appeared in the early stages of the programme. Explore actively identifies potential routes to adoption through Excelerate, while defining their own projects. Excelerate teams also identify potential adoption projects that require more early-stage research or POC work before the adoption phase. This approach has contributed to a healthy pipeline of projects from Explore to Excelerate, as was intended at the start of the programme.

[6] https://www.nafems.org/ https://www.apcuk.co.uk/

Each of the themes outlined above now has at least one project that has been carried forward to Excelerate. This includes:

- The materials platform and surrounding work is being used in an Excelerate project to prepare tools for simulating chemical structures and their properties within fuel cells.[7]
- A series of projects with REPROCELL started in Explore under the life sciences theme. The projects focused on utilising REPROCELL's access to multiomics data to generate insight into drug efficacy in different patient population and are now being finalised for adoption through Excelerate.[8]
- Explore projects with Dark Matter Labs[9] and Royal Haskoning DHV[10], respectively, are being prepared for partner or open-sourced adoption through Excelerate. The projects with Dark Matter Labs aim to project the financial and societal benefits of nature-based solutions for use in a financing platform, whereas those with Royal Haskoning DHV are developing a multi-hazard business impact service for climate resilience.

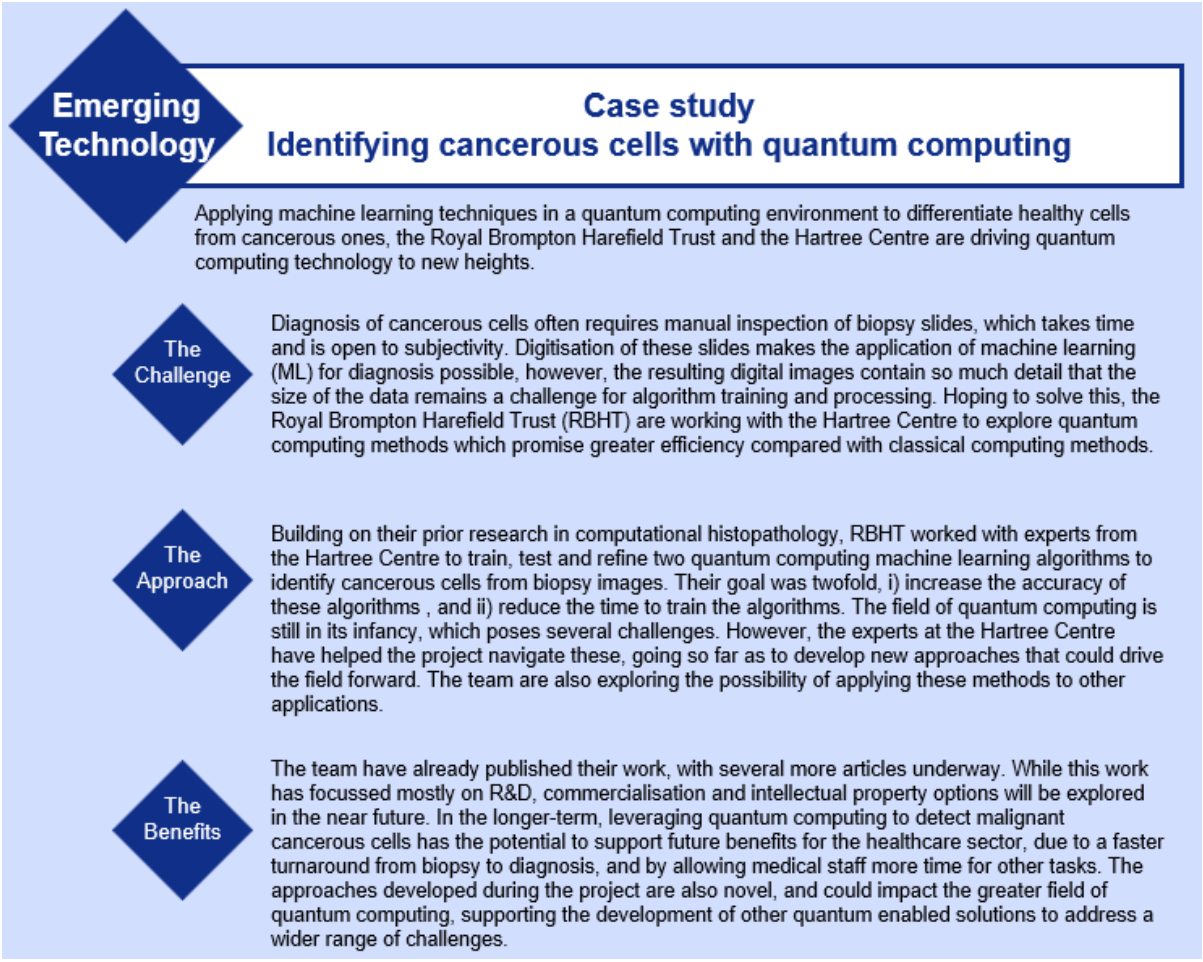


[7] https://matthey.com/

[8] https://www.reprocell.com/

[9] https://darkmatterlabs.org/

[10] https://www.royalhaskoningdhv.com/



The link to the full case study of HNCDI's work with the Royal Brompton Harefield Trust can be found here.

Excelerate

In contrast to Explore, Excelerate has set its primary focus on driving the *adoption* of digital technologies. Each Excelerate project must include an external collaborator that is interested in implementing these technologies within their organisation.

The Excelerate workstream has made substantial progress over the last year, having received additional attention over the last 18 months to clarify its messaging to potential partners and enhance internal project pipeline processes. These efforts have brought the workstream on track to achieve its targets for 2026, with 30 PMDs approved (target of 32), 15 projects in progress and 3 closed.

Since the prior reporting period, this complex workstream is better defined and the mechanics of developing software assets in partnership with industry are better understood with respect to asset ownership and licensing agreements that are attractive to project partners. The scoping of projects has been adjusted and combined with that of Explore, and the addition of dedicated resources and priority within the Project Management team has reduced the time it takes to advance an approved project through negotiations and get it started. The programme team have also been focusing on how to leverage the relationships and projects from prior HNCDI projects to identify further opportunities for application through Excelerate. This has included building positive relationships with project partners, which has in some cases resulted in additional projects e.g., the partnership with REPROCELL. Building on the success of the Emerging Technology workstream, the Excelerate team is also prepared for the possibility of quantum computing-based adoption projects identified in the extended pipeline recorded by the business development team for Excelerate. As a result, there are now over 20 additional projects in the pipeline, with the focus also on those projects that can be completed within the current HNCDI programme timeframe.

Several Excelerate projects are due to start their evaluation license periods with their respective project partners. This represents a period over which the license for assets developed with partners is granted for free, allowing the partner organisation to familiarise themselves with the asset in their own working environment and begin integrating it with their internal operations. The length of the evaluation period depends on the contract negotiated at the start of the project and this process increases the knowledge exchange between the HNCDI team and the industrial collaborator.

Complete industry adoption of digital technologies remains challenging due to hesitancy and a lack of awareness of benefits. However, Excelerate is positioned to address these challenges by supporting companies through the adoption process, mitigating some of the risks associated with developing and adopting fit-for-purpose digital technologies in-house for UK businesses.

Explore & Excelerate

Development of digital assets

Over the course of the programme, Explore has developed digital solutions across multiple areas. Several of these solutions have been taken forward and expanded in Excelerate, where they will eventually be adopted by project partners.

Polymers

Three projects from Explore – aimed at developing automated workflows for polymer simulation, virtual experiments capability, and polymer coating toolkits – have been combined to explore the properties of polymer structures. Organisations interested in using this capability have started projects through Excelerate. For example, the team are working with Victrex to model fatigue in the polymers they produce. The team are also working with Johnson Matthey to prepare tools for simulating chemical structures and their properties within fuel cells.

Omics

An Explore project for finding the best ways of modelling multi-omic data has enabled Excelerate projects with partners like 2Blades and Apnea-Tech. Excelerate is assisting TSL to incorporate ML capability into an existing platform that identifies disease-resistant genes in crops. The team are also working with Apnea-Tech to develop a model for diagnosing sleep apnoea using SpO2 levels.

Excelerate

Partner organisation profiles*

*Based on a survey of partners, n=16

Size

Most partner organisations (50%) are very small, with 1-9 employees. A further 25% of partners fall between 10-49 and 50-249 employees, and the remaining 25% comprise larger organisations consisting of more than 250 employees.

Type

Half of the surveyed partners categorise themselves as 'business or commercial' organisations. A third of partners are RTOs, 8% are 'academic or university' organisations and the remainder are 'other', meaning none of the above nor public sector categorisation applies.

Sector

Several partner organisations operate across multiple sectors each. Two thirds have activities in the sustainability sector, half are involved in innovation, a third carry out work in the health sector, and a third work in the manufacturing sector.

Expectation

Most partner organisations have no prior experience with AI or HPC. More than 80% of partners also reported that their HNCDI project was their first time working with the Hartree Centre and/or IBM. The most common outcome expected from their HNCDI projects is new/valuable knowledge to the organisation, with a strong possibility of commercial benefits.

4. Engagement – SME Hubs

Three SME Engagement Hubs were launched in the second half of 2023. They aim to assist SMEs by increasing their productivity and competitive advantage through digital technologies such as supercomputing, data science, artificial intelligence/machine learning, and visual computing.

The SME Engagement Hubs are: [11]

- **The Hartree Centre Cardiff Hub (Cardiff Hub)**, hosted by the Digital Transformation Institute at Cardiff University.
- **The Hartree Centre North East Hub (NE Hub)**, hosted by the National Innovation Centre for Data at Newcastle University and in partnership with Sunderland Software City.
- **The Hartree Centre Northern Ireland Hub (NI Hub)**, hosted by Ulster University.

The Hubs have received £4.5m in funding from government and IBM – allocated through HNCDI – over three years and leverage the expertise and support of the Hartree Centre and IBM to deliver a range of services aimed at local SMEs. The Hubs offer practical interventions in the form of short-term assists, for scoping regional needs and developing strategies to address them. In addition, they offer longer-term projects in which the Hubs collaborate with SMEs to develop ready-to-implement solutions for their business. These projects originate as follow-ons from assists or from publicised calls to which SMEs submit proposals. In total across the three hubs, they have a target of 66 projects and 170 assists over their three years of funding.

Just over a year since their launch, all three Hubs are fully operational with assists and projects progressing as expected. As of December 2024, the Hubs have delivered a total of 65 assists and 25 projects and are on track to convert enough of these assists into projects to reach their combined target by the end of the programme. SMEs from various sectors, like manufacturing, education, legal, healthcare and food, have been taken from assists through to projects. Those assists that have not been carried through as full projects have also provided SMEs with knowledge and increased capacity to move forward with their digital strategies and R&D funding applications.

The HNCDI programme does not have fixed criteria for engaging with regional SMEs. Instead, each Hub sets its own strategies and methods based on its knowledge of local landscapes and socio-economic challenges. Hub Leads agree that this flexibility has contributed to successful engagement, with each of the Hubs effectively extending the reach of the HNCDI programme beyond what had been achieved before (project applicant profiles show that most have no prior history with the Hartree Centre). The additional reach afforded by the Hubs is critical to the overall programme's goal of supporting small businesses in adopting digital technologies, since even though SMEs make up over 99% of all businesses in the UK, they remain a challenging demographic to engage, given their limited resources and networks.[12] Referrals remain a strong engagement method employed by the Hubs to reach SMEs. These referrals are routed in the hosts' existing networks and through membership organisations as well as local government initiatives with which the Hubs have partnered. Additionally, the Hubs also regularly attend and present at local sectoral events. Some of the Hubs have begun to explore other ways of reaching SMEs such as establishing collaborations in new geographical areas.

The Hubs run their own networking and knowledge exchange events, offering workshops and training opportunities locally. So far, the Hubs have held over 40 knowledge exchange events and engaged over 200 SMEs.

The Hubs also connect their networks with HNCDI's Explain training offering, allowing these networks to benefit from expertise within the wider programme for free. However, the emphasis remains on locally

[11] https://www.cardiff.ac.uk/hartree/about; https://www.hartreenortheast.uk/#meet-the-team; https://hartreeni.uk/

[12] https://www.gov.uk/government/statistics/business-population-estimates-2023/business-population-estimates-for-the-uk-and-regions-2023-statistical-release

available support, with each Hub largely leveraging its own networks and resources to reach and assist SMEs in their digital adoption journey.

Organisations supported through the Hubs' assists, projects and engagement events are already reporting positive outcomes. Organisations that engaged with the Hubs identified insufficient knowledge about digital technologies and their applicability as a major challenge to their adoption and capability building. This has historically discouraged SMEs from pursuing the uptake of digital technologies, believing they are only within reach of large companies. Following their engagement with the Hartree Centre SME Hubs, participants reported that the assists and events provided them with a practical foundation on which they can build their digital strategies. The projects have also enabled SMEs to access data science expertise and leverage their existing data to uncover insights to make informed business decisions. Interviews with the Hub leads also highlighted that projects have enabled SMEs to develop tools for improved business processes and efficiencies. Some examples of projects supported by the Hubs and benefits realised to their participants include:

- The Northern Ireland Hub worked with food manufacturer McColgan's to develop a data-driven prediction system to help them maintain a suitable inventory and minimise production waste.[13] The prediction system uses McColgan's historical data to improve the company's ability to accurately forecast product orders. William McColgan, Director of McColgan's said "we would have spent years trying to develop a solution ourselves. Working with the Hartree Centre Northern Ireland Hub allowed us to get on with the application of the model, rather than developing it ourselves from scratch."
- The Cardiff Hub worked with Rusty Design, a startup based in South Wales that specialises in design, prototyping and small-scale manufacturing, to automate the creation of objects, assign textures and create a library of digital objects for sports equipment and props for the television and film industries using generative AI.[14] The use of AI in Rusty Design's processes and workflows is intended to enable agile and sustainable production. The guidance provided by the Cardiff Hub has also helped Rusty Design acquire Innovate UK funding from the Creative Catalyst. Belddyn Williams, Director of Rusty Design said "without the support of the Hartree Centre Cardiff Hub, we wouldn't have been able to access the expertise we needed and unlock the path forward for our future projects around generative AI, readying us for commercialisation."
- The North East Hub worked with Floki Health, a healthcare technology company, to develop an interactive visualisation tool that simplifies complex data, allowing medical staff to find assets quickly and easily.[15] The tool enables medical staff to find hospital equipment quickly and potentially save time, money, and improved patient care. Fenwick Smith, Director of Floki Health said the hub "helped us to unlock the value and power of our data through a combination of visualisation and optimisation."

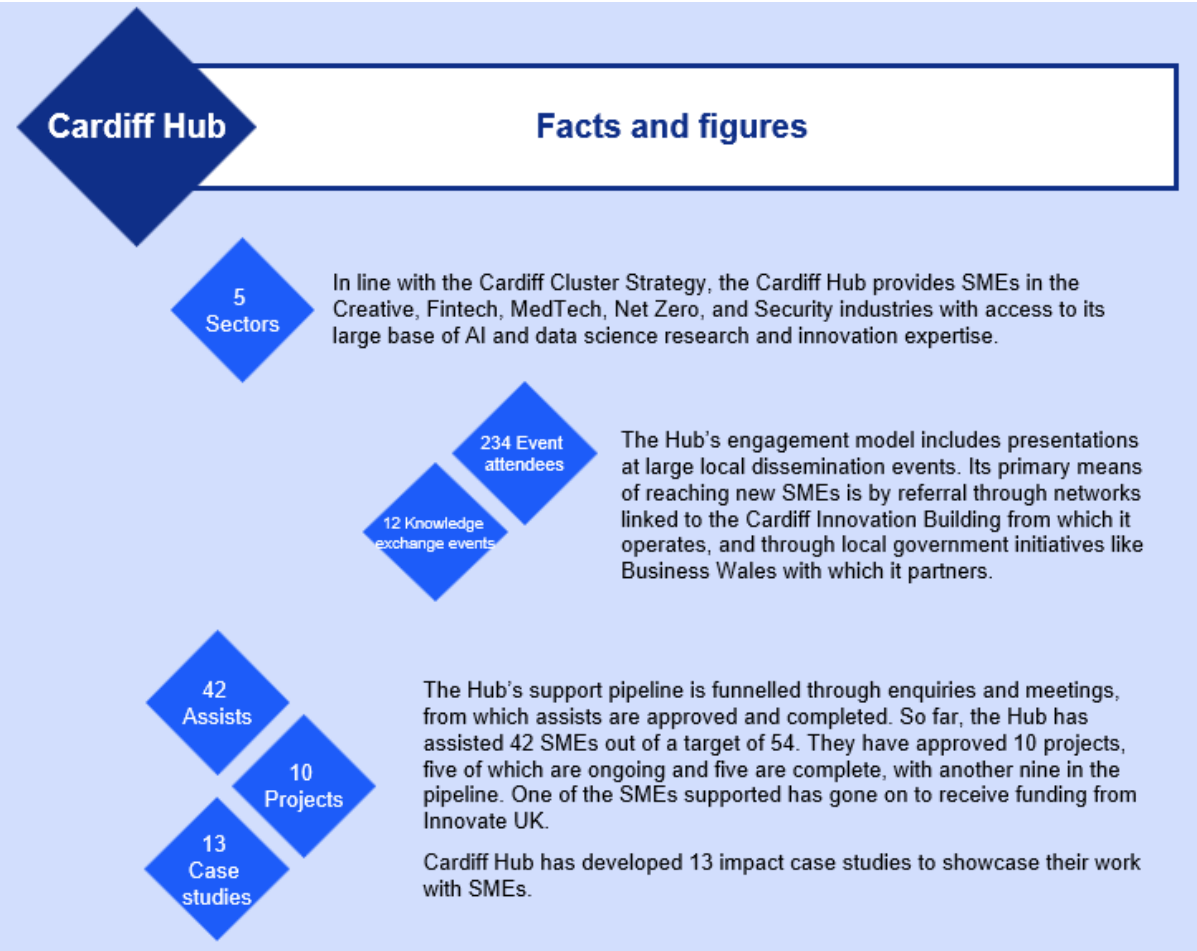
Through these collaborative projects led by the Hubs, participating SMEs have been able to learn new skills like data visualisation and increase their understanding of digital technologies. In turn, these solutions are being applied within their businesses and to future projects.

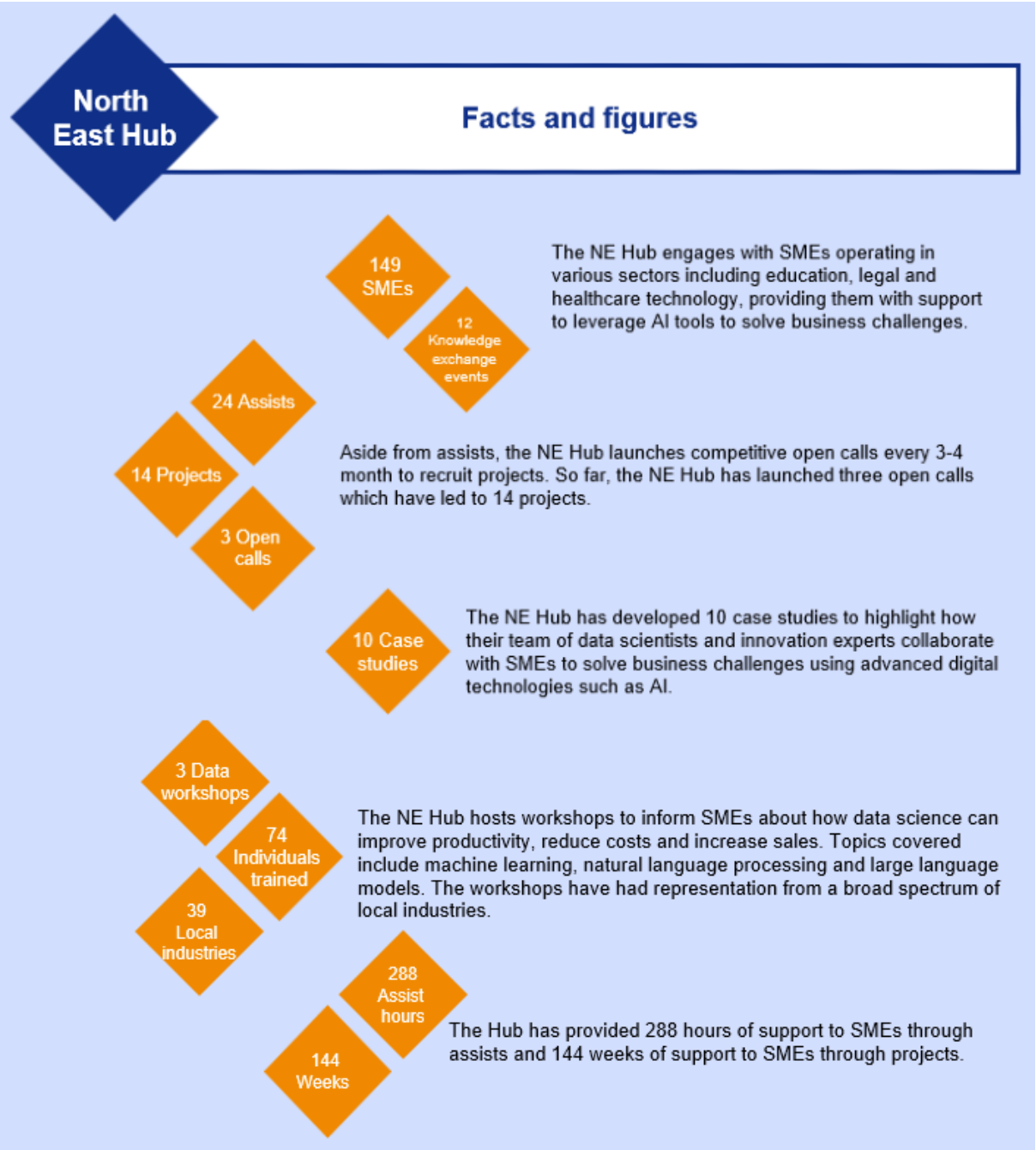
The organisations leading the Hubs are themselves benefitting from their participation in the HCNDI programme. To deliver support, programme funding has enabled these lead organisations to recruit data scientists and business development teams, increasing their overall skills and ability to serve local businesses. Indirectly, the academics involved in delivering longer-term projects also benefit from the research carried out; they have an improved understanding of the ways digital technologies can work for them, as well as opportunities for spin-off or follow-on projects. Hub activities have also led to increased awareness among SMEs of STFC and the Hartree Centre and its offerings to businesses.

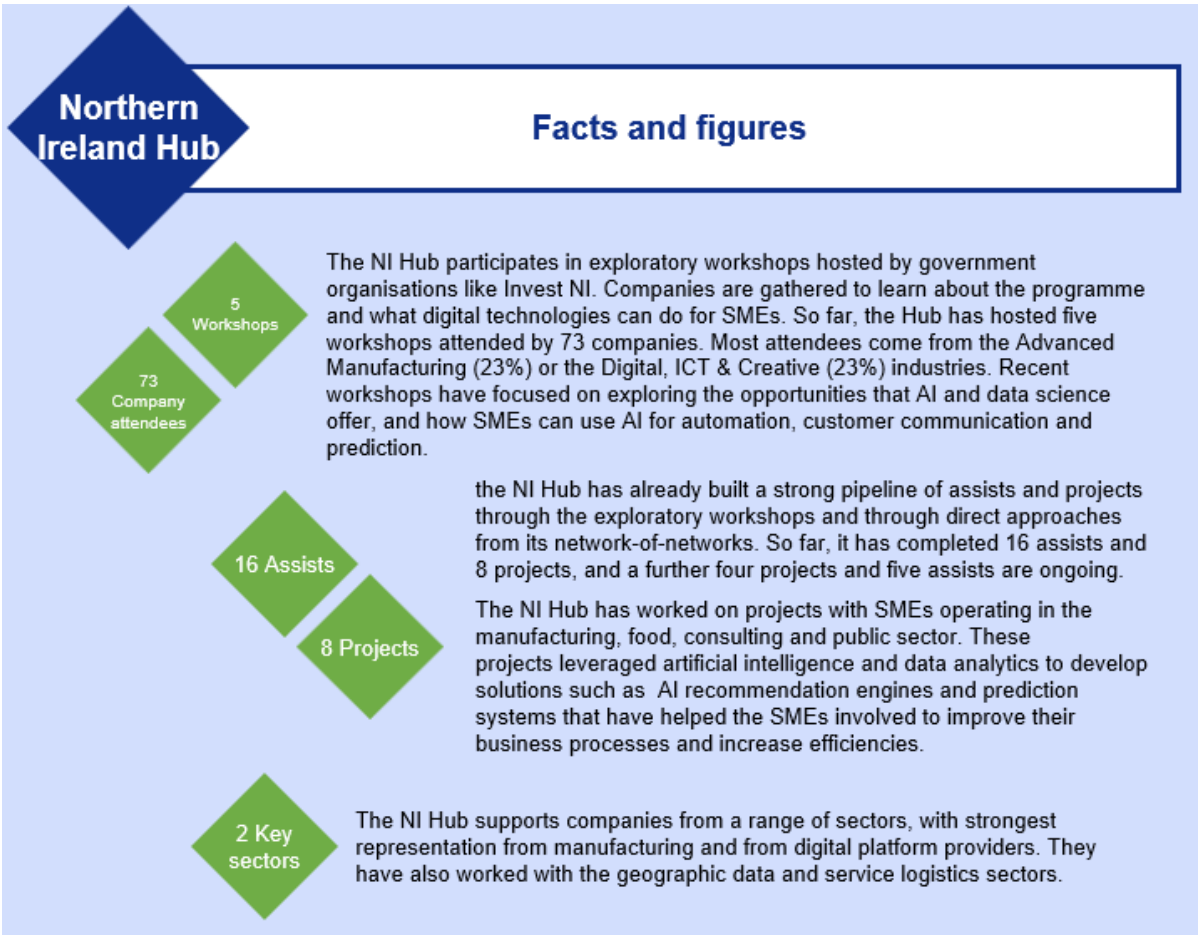
[13] https://hartreeni.uk/mccolgans_successstory

[14] https://www.cardiff.ac.uk/hartree/success-stories/rusty-design

[15] https://www.hartreenortheast.uk/insights/case-study-visualisation-and-optimisation-of-hospital-equipment


Cardiff Hub
Facts and figures
5 Sectors
In line with the Cardiff Cluster Strategy, the Cardiff Hub provides SMEs in the Creative, Fintech, MedTech, Net Zero, and Security industries with access to its large base of AI and data science research and innovation expertise.
234 Event attendees
12 Knowledge exchange events
The Hub's engagement model includes presentations at large local dissemination events. Its primary means of reaching new SMEs is by referral through networks linked to the Cardiff Innovation Building from which it operates, and through local government initiatives like Business Wales with which it partners.
42 Assists
10 Projects
13 Case studies
The Hub's support pipeline is funnelled through enquiries and meetings, from which assists are approved and completed. So far, the Hub has assisted 42 SMEs out of a target of 54. They have approved 10 projects, five of which are ongoing and five are complete, with another nine in the pipeline. One of the SMEs supported has gone on to receive funding from Innovate UK.
Cardiff Hub has developed 13 impact case studies to showcase their work with SMEs.


North East Hub
Facts and figures
149 SMEs
12 Knowledge exchange events
The NE Hub engages with SMEs operating in various sectors including education, legal and healthcare technology, providing them with support to leverage AI tools to solve business challenges.
24 Assists
14 Projects
3 Open calls
Aside from assists, the NE Hub launches competitive open calls every 3-4 month to recruit projects. So far, the NE Hub has launched three open calls which have led to 14 projects.
10 Case studies
The NE Hub has developed 10 case studies to highlight how their team of data scientists and innovation experts collaborate with SMEs to solve business challenges using advanced digital technologies such as AI.
3 Data workshops
74 Individuals trained
39 Local industries
The NE Hub hosts workshops to inform SMEs about how data science can improve productivity, reduce costs and increase sales. Topics covered include machine learning, natural language processing and large language models. The workshops have had representation from a broad spectrum of local industries.
288 Assist hours
144 Weeks
The Hub has provided 288 hours of support to SMEs through assists and 144 weeks of support to SMEs through projects.


Northern Ireland Hub
Facts and figures
5 Workshops
73 Company attendees
The NI Hub participates in exploratory workshops hosted by government organisations like Invest NI. Companies are gathered to learn about the programme and what digital technologies can do for SMEs. So far, the Hub has hosted five workshops attended by 73 companies. Most attendees come from the Advanced Manufacturing (23%) or the Digital, ICT & Creative (23%) industries. Recent workshops have focused on exploring the opportunities that AI and data science offer, and how SMEs can use AI for automation, customer communication and prediction.
16 Assists
8 Projects
the NI Hub has already built a strong pipeline of assists and projects through the exploratory workshops and through direct approaches from its network-of-networks. So far, it has completed 16 assists and 8 projects, and a further four projects and five assists are ongoing.
The NI Hub has worked on projects with SMEs operating in the manufacturing, food, consulting and public sector. These projects leveraged artificial intelligence and data analytics to develop solutions such as AI recommendation engines and prediction systems that have helped the SMEs involved to improve their business processes and increase efficiencies.
2 Key sectors
The NI Hub supports companies from a range of sectors, with strongest representation from manufacturing and from digital platform providers. They have also worked with the geographic data and service logistics sectors.

5. Training – Explain

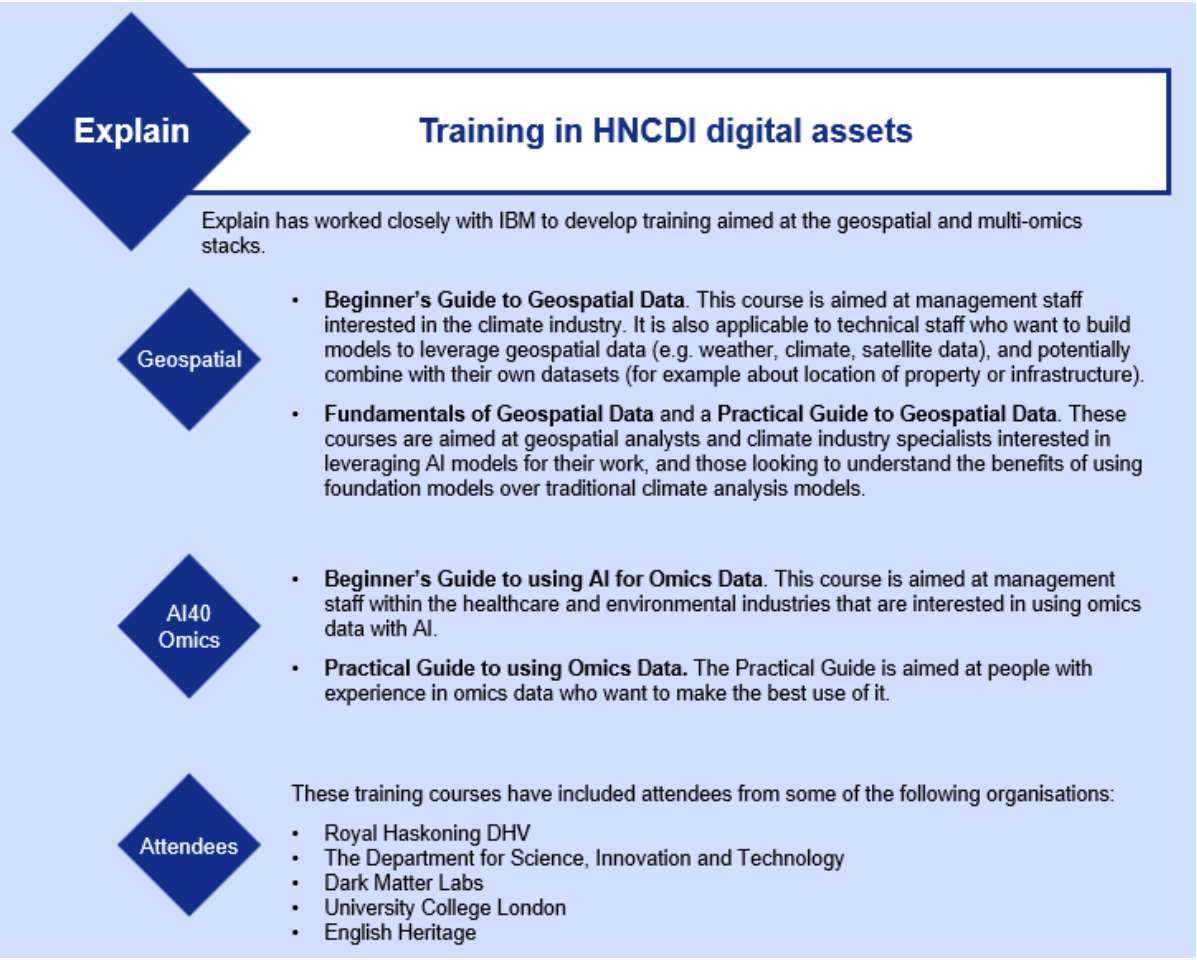
The Explain workstream develops and provides free training courses and tutor-led modules on data science aimed at industry. This focus reflects international demand for upskilling in high performance computing (HPC), particularly for senior management.[16] Explain has trained over 2,300 individuals to date; an increase of nearly 1,000 since the previous report across >900 businesses.

The programme invested heavily at an early stage to adapt content for businesses and non-academic audiences, and to make it convenient and accessible via their Learning Management System (LMS) – an online learning platform. Explain has also been working closely with the CR&D workstreams to develop targeted training related to specific assets and projects within the programme. These courses are intended to assist project partners, but they remain available to anyone through the programme's LMS. In one example, training has been developed around two of the applied technology themes (the Environment and Life Sciences) that are used in Explore and Excelerate, with the aim of increasing the likelihood of successful adoption of solutions upon project completion by upskilling adopting organisations.

The area of geospatial discovery now has three training courses available through Explain aimed at different levels of expertise: a Beginner's Guide, a Fundamental Guide, and a Practical Guide to Geospatial Data.[17] Under Life Sciences, two courses are available to explore the use of multiomics datasets. Like the training for geospatial data, multiomics courses are aimed at different knowledge levels through from Beginner's Guide to a Practical Guide to using AI for Omics Data. A third omics course about evidence of collaboration to upskill the community is due to go live in 2025. These themed courses have so far been attended by 37 individuals.

[16] https://eurohpc-ju.europa.eu/two-new-calls-support-hpc-training-activities-2023-01-31_en

[17] https://www.hartree.stfc.ac.uk/live-sessions/2024/04/17/fundamentals-of-geospatial-data/



6. E-infrastructure – Cloud, On-premise Cloud and the Supercomputing Centre

The new **Supercomputing Centre** (SCC) is expected to be fully operational and integrated with the Hartree Centre's activities by the fourth quarter of 2025. As of December 2024, the building is complete and the centre has entered a phase of testing and commissioning, with a substantial amount of mechanical infrastructure that needs to be deployed and tested in this period. This, as well as the installation of the high-performance computer (HPC), is expected to be completed in May 2025, after which it will be handed over to STFC to configure and integrate.

The SCC is the first completely new building to be constructed at Daresbury since the Hartree Centre was established, which has meant a lot of learning for the site's Estates team. To deliver a resource that might serve not only the Hartree Centre but also the wider STFC, the Estates team collaborated with several other teams and departments across the organisation and the Hartree Centre itself – to ensure a result that is fit for purpose and interoperable. There is now an opportunity for other departments at STFC to make use of the SCC for their scientific computing needs.

The centre has been fitted with equipment to monitor key variables that contribute to its energy efficiency, such as temperature, pressure, humidity and air flows. Sophisticated water cooling and building management systems have also been installed. To fully exploit these assets, the programme already has a project underway to develop a digital twin of the SCC that would optimise operating conditions. The outcome of this project could provide substantial evidence and insight into mechanisms

and approaches for increasing the environmental efficiency of other data and computing facilities across the STFC portfolio.

Furthermore, the SCC has been constructed over a period of substantial changes in the physical and cyber threat landscape. Given the Hartree Centre's close working relationship with industry partners, ensuring security of the SCC is of high importance. To account for this, the National Cyber Security Centre was consulted for modelling and risk assessment, and standard operating procedures for the SCC have been developed accordingly. These new procedures are also expected to have potential applications for other facilities across the STFC portfolio, helping to increase the security and resilience of research infrastructures in other domains as well.

In the meantime, the HNCDI programme has made good use of **on-premise** and **public cloud** services. For example, cloud access is used to de-risk projects by giving access to additional computing resources on short notice. This, in turn, has enabled the programme to explore digital technologies, for which projects require short bursts of high compute use while in development and testing. The use of public cloud providers like AWS, IBM and Azure also allows projects to be tested in the same environment that clients will use in the adoption phase of their digital solution.

Appendix – Interviews

Area of expertise	Name	Organisation
HNCDI Programme Management	Kate Royse	STFC
HNCDI Programme Management	Michael Bradley	IBM
	Peter Waggett	
HNCDI Programme Management	Sergio Malo-Peces	STFC
Emerging Technology Workstream	Stefano Mensa	STFC
	Jason Crain	IBM
Explore Workstream	Richard Anderson	STFC
	Geeth de Mel	IBM
Excelerate Workstream	Kyle Hatchard	STFC
	Christopher Gibson	IBM
E-infrastructure Workstream	David Cable	STFC
Cardiff Hub	Alun Preece	Cardiff University
	Luiza Patorski	
North East Hub	Barry Hodgson	Newcastle University
	Ashmita Randhawa	Sunderland Software City
Northern Ireland Hub	Justin Quinn	Ulster University