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HARTREE NATIONAL CENTRE FOR DIGITAL INNOVATION

PROGRESS REPORT

2024

Hartree National Centre for Digital Innovation Progress Report

For the period January – December 2023

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March 2024

Hartree Centre

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Executive Summary

The Hartree National Centre for Digital Innovation (HNCDI) utilises the powerful computing capabilities, world class expertise and one-of-a-kind infrastructures available to UK businesses and public sector organisations at the STFC Hartree Centre and in collaboration with IBM. Delivered across six core work streams, and supported by a central programme management team, HNCDI supports collaborative projects (Explore, Excelerate & Emerging Technology work streams), delivers training and SME engagement (the Explain work stream and recently launched HNCDI Hubs) and hosts a wide range of e-infrastructure.

This document presents a second progress report for the 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 in its first 30 months (to December 2023).

Having reached its mid-programme milestone, HNCDI has established all of its core workstreams of activity, is making good progress overall against its original targets, and is already delivering innovative solutions to industry challenges.

Highlights:

- One highlight of the past year is the launch of **three SME Engagement Hubs** that target regions of the UK which often struggle to access expertise in digital technologies. The three hubs are based in Cardiff, the North East of England and Northern Ireland. Each hub leverages its knowledge of local businesses to deliver assists and projects in ways that are accessible to SMEs, and their approach is yielding tangible benefits. In the short time that the Hubs have been active, over 140 organisations have already been engaged and 27 projects started. The Hubs build a digitally engaged SME network across the UK under the HNCDI programme.

- The reputation and expertise in quantum computing developed through the HNCDI programme played a key role in the decision of US quantum computing company **PsiQuantum** choosing the Sci-Tech Daresbury Campus as the location for its first R&D facility outside of the US. To leverage this HNCDI developed expertise, PsiQuantum and the Hartree Centre subsequently launched a collaborative project, funded by the National Security Strategic Investment Fund, to cultivate practical industrial applications in preparation for the advent of large-scale, fault-tolerant quantum computing (FTQC).

- Across the R&D workstreams: **Emerging Technology, Explore** and **Excelerate**, 87 projects have been launched (as of December 2023), 40 have successfully completed. In parallel, these workstreams have engaged 24 unique partner organisations and secured approximately £1.5m of in-kind contributions. The projects have started to produce codified knowledge, demonstrated in 30 peer-reviewed publications, while one patent submission is also in progress.

- Through the **Explain workstream** – hosting a dedicated platform of free training courses tailored to industry challenges – 1,340 individuals from 336 different organisations have attended. A range of industry and public sector organisations have engaged with Explain training. The courses have also been well received, with around 84% of attendees reporting that courses have improved their knowledge, and 75% reporting positive or very positive experiences about the relevance of the training provided. In addition, the success of these courses and the lessons learnt from the implementation of the workstream have attracted interest from other centres across Europe who are keen to learn from HNCDI's pioneering approach.[1]

- Another measurable highlight of the programme is the increase in STFC Hartree Centre's **e-infrastructure capacity**. Both public and on-premise cloud facilities are now fully implemented and available to HNCDI projects. The construction of the supercomputing centre also began at Sci-Tech Daresbury in January 2023 and is on track for completion in the Autumn 2024, after which the supercomputer will be available in 2025.

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[1] HPC Centre Stuttgart (HLRS). More detail can be found in the Explain section of the report.

Introduction

The Hartree National Centre for Digital Innovation (HNCDI) was launched in June 2021 to drive the research and adoption of digital technologies in the UK. 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.

More than two years into the programme, it remains as relevant now as at its inception. The UK Science and Technology Framework, published in 2023, identifies both AI and quantum technologies as two of the five critical technologies for the UK to intensify between now and 2030.[2] HNCDI is a key contributor to addressing that challenge, providing training and access to the computation facilities of both the Hartree Centre and the IBM Quantum Network, as well as access to the specialist knowledge and expertise of their staff.

The HNCDI programme employs a multi-layered approach to supporting R&D and the adoption of AI and quantum computing technologies. To deliver against its aims, the programme is comprised of five activities to address key stages of digital adoption:

Explain

Aims to provide accessible and application focused training courses that span a range of digital economy topics, such as AI, machine learning, high performance computing and quantum computing. Courses are presented in a variety of formats, from self-paced e-learning to live sessions.

Explore

Develops proof-of-concepts that target the frontier of AI and digital technologies. Real-world challenges are identified and solutions with high potential value to industry are developed in collaboration with industry users.

Excelerate

Applies research and innovation to turn good ideas into industry-ready solutions that address key challenges. Working closely with businesses, this workstream lowers the barriers to innovation to create enhanced products and services and generate long-term societal and economic impact.

Emerging Technology

Combines established high-performance computing techniques with emerging technologies like quantum computing, this workstream aims to improve the understanding around their potential for industry application.

SME engagement

The HNCDI programme has established three SME Hubs in collaboration with delivery partners. The Hubs engage with SME communities across the UK to start their digitalisation journey and deliver short projects/interventions and training.

These workstreams are underpinned by two further strands of activity:

E-infrastructure

The procurement and construction of a new energy-efficient supercomputing centre at STFC's Daresbury Laboratory, the provision of a new AI-optimised supercomputer, the procurement, and delivery of a hybrid cloud platform.

Programme management

Supports programme delivery through project management, programme monitoring, evaluation and communications activities, plus cross-programme activities, including recruitment and running seminars and workshops outside of workstreams.

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[2] https://www.gov.uk/government/publications/uk-science-and-technology-framework/the-uk-science-and-technology-framework

This report and methodology

This document presents the second of three progress reports for the HCNDI programme. It focuses on developments and emerging results for the period following the first progress report (June 2021 – December 2022) until December 2023. The methodology used to prepare this report has been aligned with the objectives set out in the Evaluation Framework Report (May 2022), and combines:

- **Desk research and review of programme documentation** – Programme monitoring information including HNCDI KPIs, project management documents (PMDs), and survey feedback were shared by the HNCDI team and reviewed by the study team.

- **Stakeholder interviews** – A series of four interviews were conducted with the programme delivery team. These focussed primarily on the three SME Hubs which were launched after the first progress report. A separate interview was conducted to gather information on the evolution of the Emerging Technology strand. The list of interviewees is presented in the Appendix – Interviewees.

- **Case study summaries** – A set of three case studies focussing on projects and participants engaged in two of the programme's workstreams (Explore and Excelerate) were developed in the fourth quarter of 2023 (based on desk research, analysis of project monitoring information and interviews). The key objectives, activities and outcomes from these cases have been summarised for this report.

- **Regular conversations with the Impact Evidence and Evaluation Manager –** Fortnightly online meetings were held 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 HNCDI **SME Engagement Hubs**, their implementation and emerging benefits.

- **Section 4** presents the progress of the programme's collaborative R&D (CR&D) strands – **Emerging Technology, Explore** and **Excelerate** – including key outputs and outcomes of the programme to-date, and case studies to highlight some of the impacts emerging from these strands.

- **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**.

HNCDI Programme Progress Overview

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

For IBM, HNCDI forms part of the Discovery Accelerator initiative (the first in Europe) that builds on a previous programme entitled 'Innovation Return on Research (IROR)' that was also in collaboration with the Hartree Centre.[3]

HNCDI is now at its **halfway mark** and the programme has advanced substantially since our first progress report.[4] The potential of the programme to expand its quantum computing capabilities and deliver knowledge exchange to SMEs in regions across the breadth of the UK is clear from the evidence provided.[5]

The programme continues to **recruit new experts and upskill the teams** of the Hartree Centre and IBM, with 76 staff employed to deliver the programme's activities. In spite of concerns globally about the competition for skills and recruitment in the area of digital technologies, the HNCDI programme has surpassed its recruitment targets, having so far employed 44 staff within the Hartree Centre (target of 25) and 32 within IBM Research UK (target of 30). The collection of knowledge and skills built for the programme actively adds value to the UK's digital sector.

The HNCDI programme has principally **strengthened the collaboration between the Hartree Centre and IBM**. Projects include staff from both teams, resulting in a mutual understanding and increased appreciation of their complementary skills and capabilities. The assets of both parties continue to be leveraged, such as the Hartree Centre's Osprey cloud computing platform and IBM's Geospatial Discovery Network.[6] The programme is also resulting in shared assets such as a series of technology stacks to tackle challenges related to materials discovery for example, each developed under the Explore workstream. As part of the HNCDI programme, the Hartree Centre has also joined the IBM Quantum Network, securing access to IBM's quantum computers and development tools via the IBM Hybrid Cloud, significantly broadening the scope of industrial challenges that can be addressed.

Programme workstreams are also collaborating effectively and complementing each other. For example, insights from Emerging Technology and Explore projects

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[3] https://research.ibm.com/blog/stfc-discovery-accelerator

[4] https://www.hartree.stfc.ac.uk/publications/impact/2023/05/17/hartree-national-centre-for-digital-innovation-progress-report/

[5] https://www.psiquantum.com/

[6] https://research.ibm.com/publications/establishing-a-geospatial-discovery-network-with-efficient-discovery-and-modeling-services-in-multi-cloud-environments
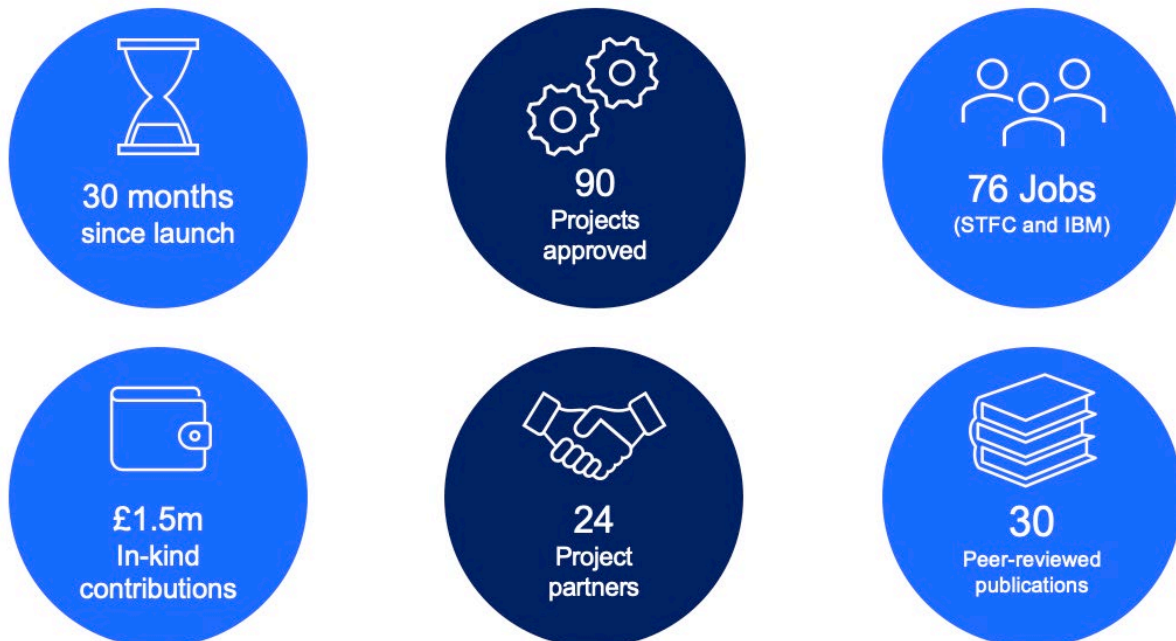
have informed some of the training developed through the Explain workstream, which in turn is offered to programme staff alongside industry counterparts, to continuously expand the knowledge and skillset of the public sector. The Explore and Excelerate strands collaborate to develop and launch calls to industry for addressing sector-specific challenges. These calls have already resulted in projects and enhanced the strategic focus of the two strands.

The programme is also enabling **new types of collaboration and support** to be delivered by the Hartree Centre which has provided valuable insights and learnings for how to better support collaborators in future. For example, the Explain workstream has been an asset to the SME Hubs, who identified a key barrier to the adoption of digital technologies by SMEs is their lack of understanding about how these technologies can be implemented into their business. Explain has several courses aimed at this beginner audience, and the Hubs report that they regularly refer companies to the training as a profound resource for upskilling.

HCNDI
facts and figures since the programme's launch

30 months
since launch

90
Projects
approved

76 Jobs
(STFC and IBM)

£1.5m
In-kind
contributions

24
Project
partners

30
Peer-reviewed
publications

Engagement – SME Hubs

Following a competitive application process, three SME Engagement Hubs were launched in the second half of 2023. These are:

- **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.[7]

The Hubs leverage the expertise and support of the Hartree Centre and IBM to deliver a range of services aimed at SMEs. They offer practical interventions in the form of short-term assists, for scoping the SME's needs and developing strategies to address them. Also on offer are 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 aggregate, the Hubs have a target of 66 projects and 170 assists over their three years of funding.

The Hubs participate in networking and knowledge exchanges, offering workshops and training events locally while simultaneously granting their networks access to HNCDI's Explain training offering. In this way, they benefit from the more established strands. However, the emphasis remains on locally available support, with each Hub largely leveraging its own networks and resources to reach and assist SMEs in their region.

The HNCDI programme has not prescribed any fixed criteria for engaging with SMEs. Instead, each Hub has the freedom to set its own strategies and methods for doing so, using their knowledge of local landscapes. 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 SMEs in adopting digital technologies, since even though they make up over 99% of all businesses in the UK, they remain a challenging demographic to engage, given their limited resources and networks.[8] Among the engagement methods employed by the Hubs are referrals routed in the hosts' existing networks and through membership organisations as well as local government initiatives with which the Hubs have partnered. They also regularly attend and present at local sectoral events.

Less than six months after their launch, the Hubs are already having a positive impact on the organisations supported through assists, projects and training. Participant SMEs surveyed have identified one of their key challenges as simply not knowing what the options and their applicabilities are when it comes to digital technologies – SMEs are often discouraged from pursuing these technologies, believing they are only within reach of large companies. These same SMEs indicate the effectiveness of the assists and events in providing a practical foundation on which they can build their digital strategies.

In addition to the impact on local SMEs, the organisations leading the Hubs are themselves benefitting from their participation in the HCNDI programme. To deliver support, programme funding has enabled the 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 the 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.

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

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

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Overall, all three Hubs regularly collaborate, sharing insights and challenges with each other to improve their own services and engagement strategies. Combined, 27 short assists and 10 projects have commenced.
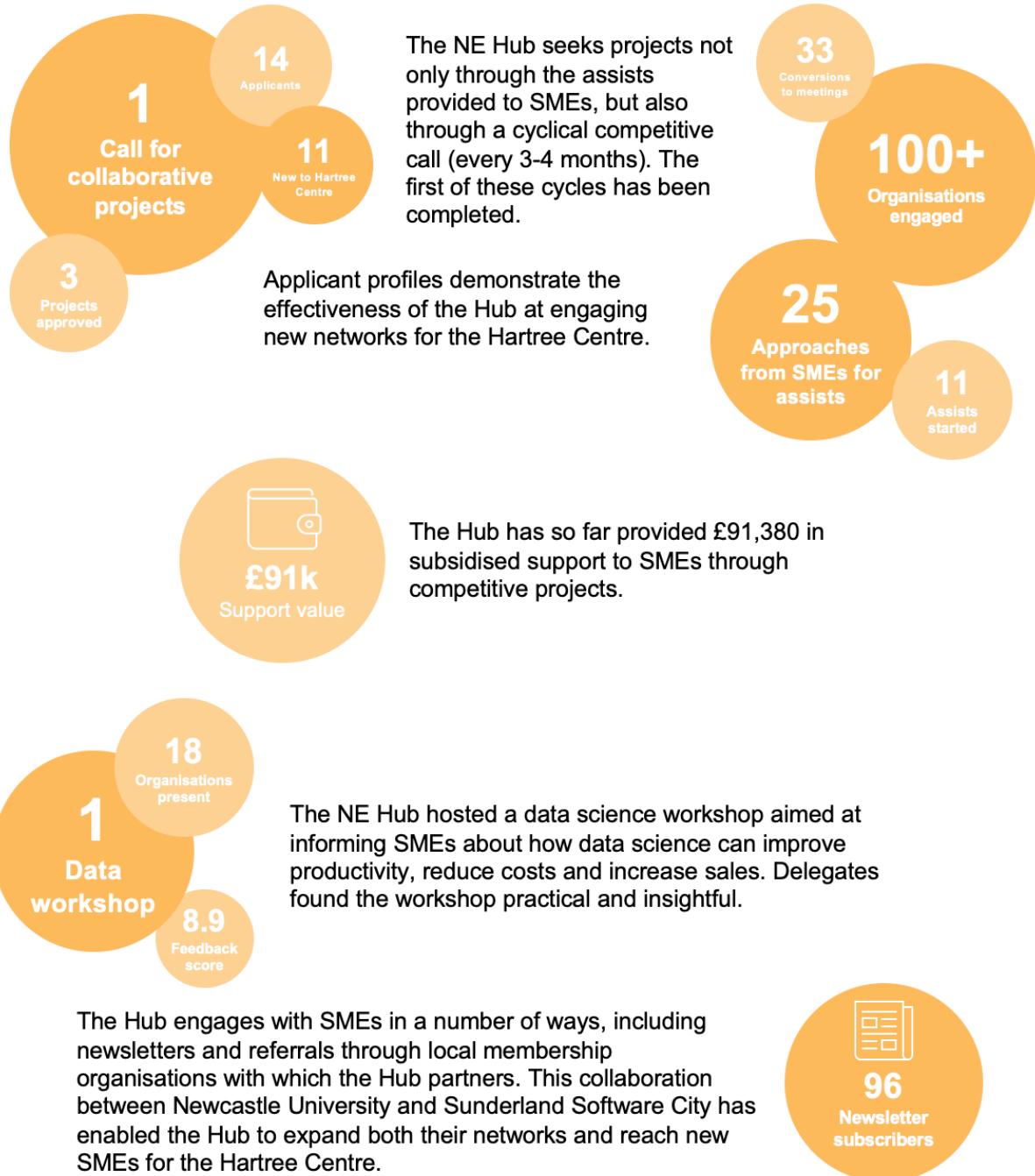
Cardiff Hub
Facts and figures

Since its launch in the second half of 2023, the Cardiff Hub has been ramping up its capacity to assist local SMEs. The full team is now onboard, including four data scientists.

11
Team members

Wales Tech Week

Welsh Govt & Google sponsored Cwmpas event

2
Large local dissemination 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.

40
The number of enquiries received from SMEs

30
Conversions to meetings

The Hub's support pipeline is funnelled through enquiries and meetings, from which assists are approved and completed. Assists will in some cases be converted to projects. The initial set of assists is expected to yield up to six projects.

6
Assists approved

3
Completed so far

The Hub's sectoral focus is in line with the Cardiff Capital Region's cluster strategy, though it will serve SMEs from any sector. Alignment with the Region's clusters streamlines the Hub's networking activities, and demonstrates local growth as its key priority.

FinTech

Net Zero

5
Sector themes, in line with the Cardiff Cluster Strategy

Creative

MedTech

Cyber-security

*https://www.cardiffcapitalregion.wales/news-events/latest-news/a-new-head-at-the-heart-of-innovation-clusters/

North East Hub
Facts and figures
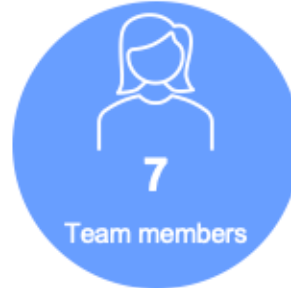
14 Applicants

1 Call for collaborative projects

11 New to Hartree Centre

3 Projects approved

The NE Hub seeks projects not only through the assists provided to SMEs, but also through a cyclical competitive call (every 3-4 months). The first of these cycles has been completed.

Applicant profiles demonstrate the effectiveness of the Hub at engaging new networks for the Hartree Centre.

33 Conversions to meetings

100+ Organisations engaged

25 Approaches from SMEs for assists

11 Assists started

£91k Support value

The Hub has so far provided £91,380 in subsidised support to SMEs through competitive projects.

18 Organisations present

1 Data workshop

8.9 Feedback score

The NE Hub hosted a data science workshop aimed at informing SMEs about how data science can improve productivity, reduce costs and increase sales. Delegates found the workshop practical and insightful.

The Hub engages with SMEs in a number of ways, including newsletters and referrals through local membership organisations with which the Hub partners. This collaboration between Newcastle University and Sunderland Software City has enabled the Hub to expand both their networks and reach new SMEs for the Hartree Centre.

**96** Newsletter subscribers

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Northern Ireland Hub
Facts and figures

As of December 2023, the NI Hub is properly established, including a full staff complement (with two data scientists), branded space at the university and a Hub website.

7
Team members

40+
SMEs engaged through workshops

The Hub participates in exploratory workshops hosted by government organisations like Invest NI (soon the Hub will host its own workshops). Companies are gathered to learn about the programme and what digital technologies can do for SMEs. These workshops include mini one-on-one interventions.

7
Leading to projects

10
SMEs receiving assists

Through the exploratory workshops and direct approaches from its network-of-networks approach, the Hub has already built a strong pipeline of assists. The majority of these assists have or will be converted into projects.

1
Project completed
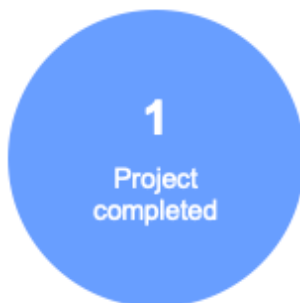
One project, related to AI vision, has been completed. The Hub assisted an SME in developing code for pattern recognition which improved what the company had been able to achieve prior to this collaboration.

Collaborative R&D Projects – Emerge, Explore, Excelerate

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

Across these workstreams, the HNCDI programme has **approved 90 projects**, an increase of 46 since the last progress report (December 2022). Of the 90 approved projects, 40 have successfully closed, with a further 38 ongoing. Eight projects are awaiting kick-off, while four will no longer be taken forward. Collectively the three strands have a target to close 156 projects by the end of the programme (June 2026).

For Emerging Technology and Explore, the number of projects closed is in line with or exceeds the target set for the 30-month point (December 2023). The Excelerate workstream is currently behind its mid-point target, having closed two projects (rather than the 10 expected). Excelerate has however seen an increase in projects starting over the past six months, with 15 projects now approved and in progress. These projects will close towards the end of the programme.

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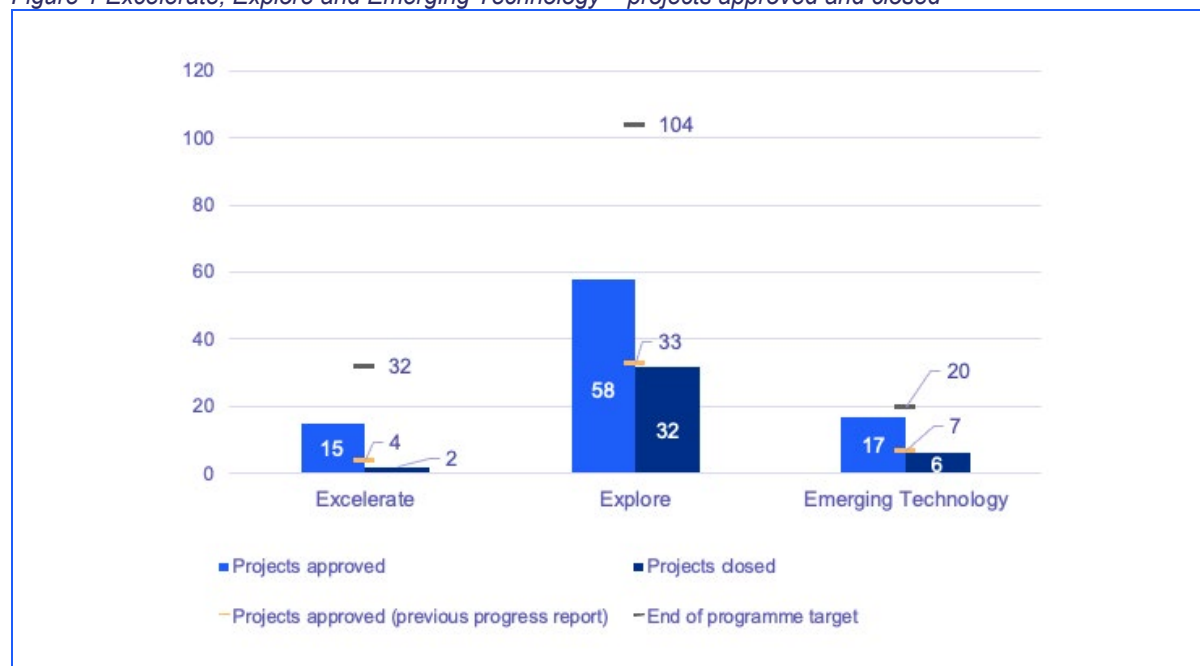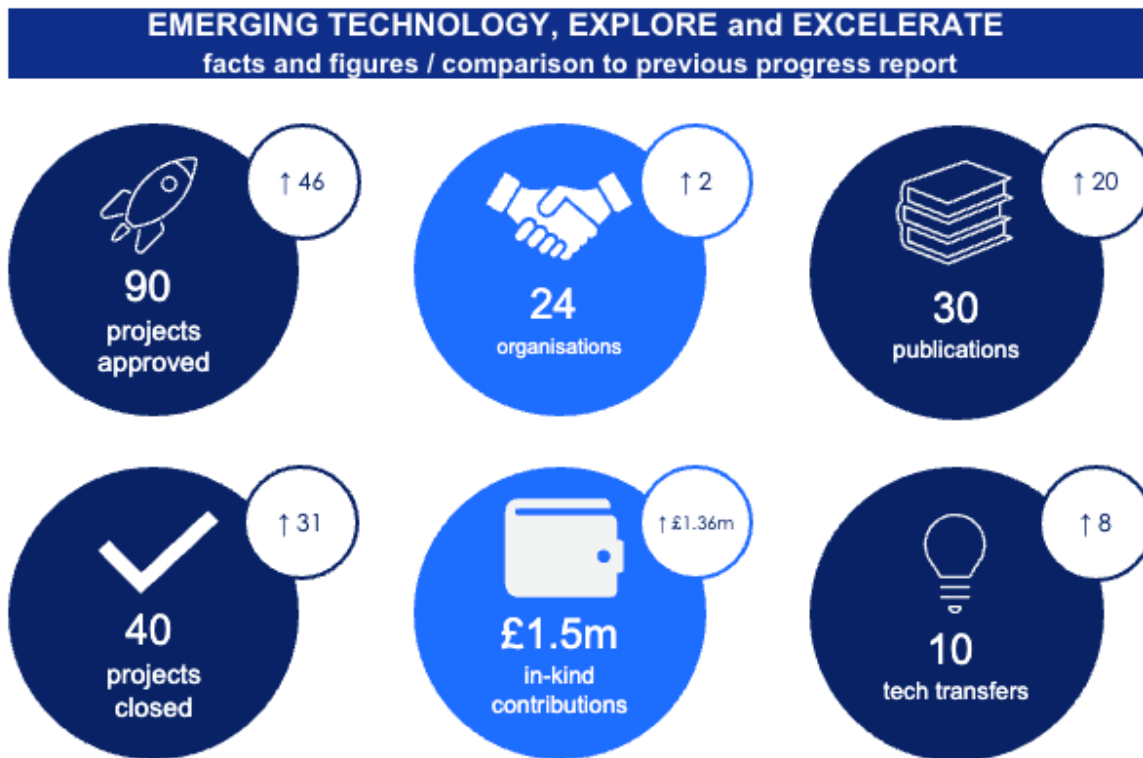

Source: HNCDI monitoring data.

The three workstreams have so far engaged **24 partner organisations** from a variety of sectors and spanning a range of different sizes. The three workstreams have also secured approximately **£1.5m of in-kind contributions** from these partner organisations – an increase of over £1.3m since the 18-month progress report. This acceleration in investment demonstrates the value of collaborative R&D carried out through HNCDI.[9]

The HCNDI programme's production of new codified knowledge has also more than doubled since the last report, evidenced for example by **30 peer-reviewed publications**. Technology transfer has accelerated as well, growing from two instances in the last report to ten as of December 2023. This technology transfer has resulted in greater insights and upskilling for core project teams, developing

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[9] 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.

novel understandings of the data organisations hold in various sectors for the UK economy. The programme is also developing tools that reusable and transferrable, with 16% of ongoing projects redeploying software assets developed in other parts of the programme.

EMERGING TECHNOLOGY, EXPLORE and EXCELERATE
facts and figures / comparison to previous progress report

- ↑ 46 — 90 projects approved
- ↑ 2 — 24 organisations
- ↑ 20 — 30 publications
- ↑ 31 — 40 projects closed
- ↑ £1.36m — £1.5m in-kind contributions
- ↑ 8 — 10 tech transfers

Source : HNCDI monitoring data

Emerging Technology

Through HNCDI Emerging Technology projects, the Hartree Centre has been building a strong reputation in the area of quantum software development. The level of industrial interest in the emerging technologies of HNCDI has been unprecedented, but also translates directly into a breadth of projects with industry and public sector partners, including the likes of the NHS and AstraZeneca, some of which have potential for follow-on developments under Excelerate. The team also published 9 papers in 2023 – one of which was the most read article in the jounal' IOPscience': *Machine Learning: Science and Technology* that year – with more currently in development.

Thanks to its growing presence, the Hartree Centre is helping to grow the emerging quantum computing sector in the North West of England, with increasing interest from quantum computing hardware and software providers who are looking to leverage the Centre's expertise and networks.

The insights gleaned by the HCNDI programme, have played a key role in opening collaboration with PsiQuantum. The most recently opened an advanced R&D facility at Sci-Tech Daresbury in 2023 and have since engaged with the Hartree Centre to support training and knowledge exchange. For PsiQuantum, a quantum computing hardware company, this is their first office outside of the US. As a result of the collaboration between IBM and the Hartree Centre and the expertise developed through HNCDI, PsiQuantum and the Hartree Centre have also launched a 12-month collaborative project. This project is funded through the National Security Strategic Investment Fund and is aimed at cultivating practical industrial applications in preparation for the advent of large-scale, fault-tolerant quantum

computing (FTQC). In future, the emergence of FTQC machines will make quantum methodologies more reliable and more generalisable to a wider range of potential applications. The project builds on the Hartree Centre's industrial network and experience in developing solutions for commercial challenges. This project is also supported by access to STFC's liquid-helium cryogenic plant – one of the largest in Europe – and a key factor in PsiQuantum's decision to base their facility at Sci-Tech Daresbury.[10]

The size of the Emerging Technologies team has grown at a rapid pace to keep up with demand for projects, and now includes 10 quantum software engineers based at the Hartree Centre. The number of staff within IBM's UK and Ireland team has also grown from a handful of people into double figures, driven in large part by the success of the HNCDI's quantum projects. To meet the growing demand for skills in quantum software development, the Emerging Technology workstream is not only training staff in a wide range of new technical skills but also exploring pathways to support new talent by looking to partially fund PhDs in future.

In late 2023, the Advanced Computing and Emerging Technologies team at the Hartree Centre were invited by IBM to become a partner in maintaining their open-source repository of quantum software for quantum machine learning applications, Qiskit Machine Learning. With around 28,000 downloads from the repository per month, the Hartree Centre is centrally positioned to provide greater support to the wider community of researchers and innovators looking to apply quantum technologies to machine learning applications, as well as playing a central role in the development and optimisation of algorithms in the coming years. This not only reflects the high calibre of work being delivered by the HNCDI team, but also the growing role the Hartree Centre can play in supporting the development of the quantum computing ecosystem internationally going forward.

As of December 2023, 17 projects have been approved under this workstream. As such, only 30 months into the programme, Emerging Technology is already 85% of the way toward its end-of-programme goal of 20 projects. Of the projects approved, 6 projects have successfully closed.

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[10] https://www.hartree.stfc.ac.uk/news/2023/10/04/psiquantum-partners-with-hartree-centre-to-develop-quantum-computing/

Explore

The Explore workstream actively supports the development of new, fundamental capabilities and application prototypes (proofs of concept). It has two core objectives: to identify early-stage digital technologies with strong industry potential, and to develop stacks of complementary projects and solutions which, when used together, offer value greater than the sum of their parts.

To identify early-stage technologies with applications that are relevant to industry, Explore has run a series of calls for proposals, each relating to a particular sector (for example automotive).[11] STFC, IBM and a sector representative collate promising projects and compile an industry challenge statement. UK businesses are then invited to match their particular challenges to the early-stage solutions set out in the call, which in turn ensures alignment of R&D to real use cases and applications.

Two calls have been completed; one for materials and one for the automotive sector, which together have resulted in four projects. Sectors that will be targeted through future calls include nuclear and energy networks, health and social care, logistics and supply chain, and Agri-tech.

Explore has so far developed three technology stacks which, in some cases, also bring together projects supported by the Excelerate workstream, including:

- A materials simulation platform which uses data on the properties of known materials to predict the characteristics of simulated materials. Using Machine Learning (ML), the platform automates 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).

- A microbiome/multi-omics software stack that uses large datasets of genetic information and combines this with other related intelligence, such as the prevalence of disease in human or animal tissue, or carbon content in soil. This supports applications in personalised medicine and environmental sciences as an example.

- A geospatial software stack, hosting a platform that combines environmental datasets, including different kinds of satellite images and geolocation data. When integrated with AI and ML, the platform has the ability to map climate change weather events such as flooding, and predict the impact of these events (for examples see the TreesAI and Riskaware impact spotlights below).

The capabilities developed within Explore are not limited to these stacks, and projects regularly innovate to build new tools with highly generalisable capability. For example, a Variational Exploration Model (VEM) was developed for Riskaware, an incident modelling software company, can be applied in any sector or situation where the outcome of a process is sensitive to a large number of variables.

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[11] https://www.hartree.stfc.ac.uk/explore/2023/02/28/automotive-call/

TreesAI
Impact from Explore

TreesAI

A collaboration led by Dark Matter Labs and Lucidminds

The challenge

The TreesAI collaboration are developing a Green Urban Scenarios (GUS) platform to drive investment in nature-based solutions (NBSs) to urban issues.

The platform must demonstrate, for example, how planting a single tree in a specific location can affect a city's resilience to flooding, and the resulting benefits to council budgets.

Due to climate change, flood damage is projected to cost the region £100m a year by 2050*

The solution

The HNCDI team enhanced and integrated its flood risk model, developed under a preceding Explore project, with GUS. This enables GUS to generate maps which highlight areas at risk of flooding based on projected rainfall patterns and existing urban topography, and simulate how these risks change with the addition of trees. The team's work also enabled GUS to estimate damages and costs for each risk scenario.

TreesAI is being piloted with the Glasgow City Council, who aim to plant 18m trees in the coming decade

Planting trees can reduce the impact of storms on human lives and infrastructure by slowing the flow of rainwater, absorbing the excess and by reducing erosion

The impact

GUS's capabilities will be used as part of the TreesAI initiative to help city councils build strong business cases for NBSs – it is currently being piloted in Glasgow, with more cities showing an interest. TreesAI supports the planning and financing of urban forests to mitigate climate risks.

* Source, https://www.glasgow.gov.uk/index.aspx?articleid=29833

Riskaware
Impact from Explore

Riskaware
A Bristol-based software company specialised in incident modelling

The challenge

Riskaware have developed Urban-Aware, a platform capable of modelling the evolution and impact of chemical plumes in built-up areas.

The company wanted to understand how the different variables used to model plume dispersion affect the speed and behaviour of Urban-Aware.

Subscribers include governments and charities

The solution

The HNCDI team used their GeoDN framework to run thousands of Urban-Aware's plume dispersion model simulations in parallel. The team developed a Variational Exploration Module (VEM) to automate the analysis of simulation data and detect patterns in the model's reaction to different combinations of variables.

Urban-Aware is used for emergency response and defence intelligence

Urban-Aware uses more than 70 variables to model plume dispersion, including urban topography and wind speed

The impact

Riskaware can use the knowledge gained from this project to improve Urban-Aware's code, as well as their own computational specifications. They also plan to use GeoDN's simulation data to develop a lighter version of the plume dispersion model for rapid response.

More generally, VEM can be used to improve very large models, like those used to design nuclear fusion experiments.

Excelerate

The Excelerate workstream's primary focus is accelerating the *adoption* of digital technologies. Accordingly, each project must include an external collaborator who will implement the technologies within their organisation. In launching Excelerate projects, the Hartree Centre and IBM have worked hard to navigate the legal challenges relating to collaborations of this nature. In doing so, both organisations have developed solutions for maintaining a strong pipeline of potential projects and collaborators to engage with, HNCDI as the programme continues.

The workstream has launched fewer projects so far than was originally forecast at the outset of the programme. However, programme management have reprofiled several aspects of the workstream to help attract new collaborators and reduce bottlenecks associated with getting those collaborators onboard. This includes the addition of a dedicated HNCDI Business Lead alongside a programme manager, earlier inclusion of legal teams in the contracting process, and a simplified presentation of legal terms.

These adaptations are already paying off, with the number of approved projects increasing from only four at the time of the last progress report, to 15 as of December 2023.

Agile Life Sciences
Impact from Excelerate

Agile Life Sciences
A start-up based in the North West of England

The challenge

Agile Life Sciences (ALS) have developed a non-invasive test to accurately identify a woman's menopausal stage from their microbiome data, called MenoGuide.

The company needed a solution to build their capacity to analyse sample data and manage customer-facing capabilities.

Tests can be invasive and imprecise

Menopause costs the UK economy up to £10bn per year in time off work*

The solution

The Hartree Centre's Research Software Engineering (RSE) team worked with ALS to digitise and integrate what was previously a disaggregated set of manual processes. The resulting platform is cloud-based, and with the help of the IBM team, it incorporates machine learning to deepen insights from sample data.

Identifying menopausal stages helps make better treatment decisions

The impact

The Menoguide platform developed under Excelerate enables ALS to commercialise and scale up their service, and to explore novel science with the platform's insights.

By making it simpler for women and their general practitioners to precisely identify menopausal stages, ALS and Menoguide can help navigate a condition that affects all women.

*Source, https://www.balance-menopause.com/news/menopause-cripples-the-uk-economy/

Explain

The **Explain workstream** develops training aimed at mid-career professionals, with a programmatic goal of delivering formal courses to **5,000** individuals by 2026 (the end of the programme). A variety of training courses have been created spanning five technology themes (HPC and Exascale, Data Science, Software Engineering, Hybrid Computing, AI Modelling) and offered at three skill levels (Introductory, Learner, Intermediate).

Explain's focus on mid-career training reflects international demand for upskilling in high performance computing (HPC), both at the practitioner level and for senior management.[12] The latter is crucial for decision-maker buy-in; training that demonstrates the applicability of HPC and related skills to their use-cases can nudge companies toward investing in the capability required.[13] With this in mind, the programme invested heavily at an early stage to adapt content for businesses and non-academic audiences.

This approach has paid off. Of the organisations registered for courses, 45% are businesses and 33% are other non-academic users. This contrasts with comparable HPC courses which attract mostly academic participants. For example, the HPC Centre Stuttgart (HLRS), which has traditionally offered training tailored to academics, launched its Supercomputing Akademie for industry in 2018.[14] HLRS have sought advice from Explain to reach similar levels of business participation. Similarly, the training offering has also attracted interest from representatives from supercomputing centres in Finland, who want to learn how their courses can appeal to industry users.

The launch of a learning management system (LMS) – an online learning platform – in October 2022 has been a key facilitator in extending Explain's reach, with over **1,340 individual attendees** recorded on training courses. This includes a significant minority of participants from outside the UK, particularly from the US, Europe and Australia, but also a small number from Asia, South America and Africa.

Explain also caters to STFC and IBM's internal training needs for topics covered under the HNCDI programme and its projects. These two organisations make up 5% of accounts registered for courses on the LMS, which demonstrates the trust they have in the programme's training.

High levels of approval are reported by attendees of Explain courses, with 84% of survey respondents stating that their knowledge had improved as a result of this training, and 75% expressing that they found the courses relevant to their work (see Figure 2).

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[12] https://eurohpc-ju.europa.eu/two-new-calls-support-hpc-training-activities-2023-01-31_en
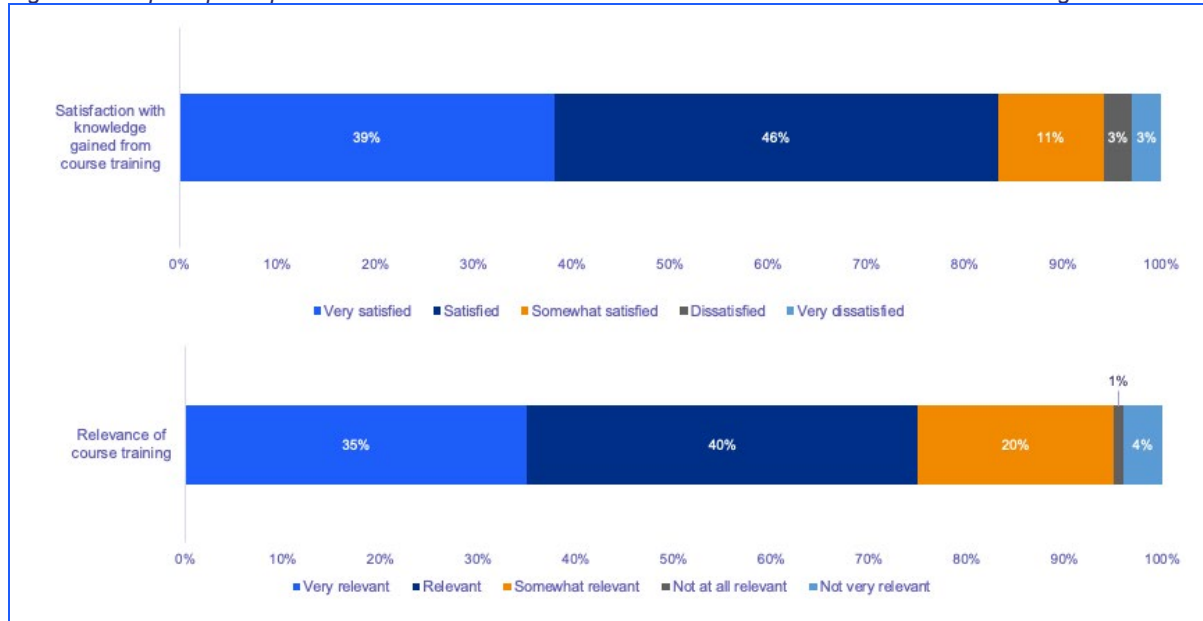
[13] https://www.scientific-computing.com/news/high-demand-supercomputing-skills-ichec

[14] https://www.hlrs.de/news/detail/the-supercomputing-akademie-a-new-hpc-training-program-opens
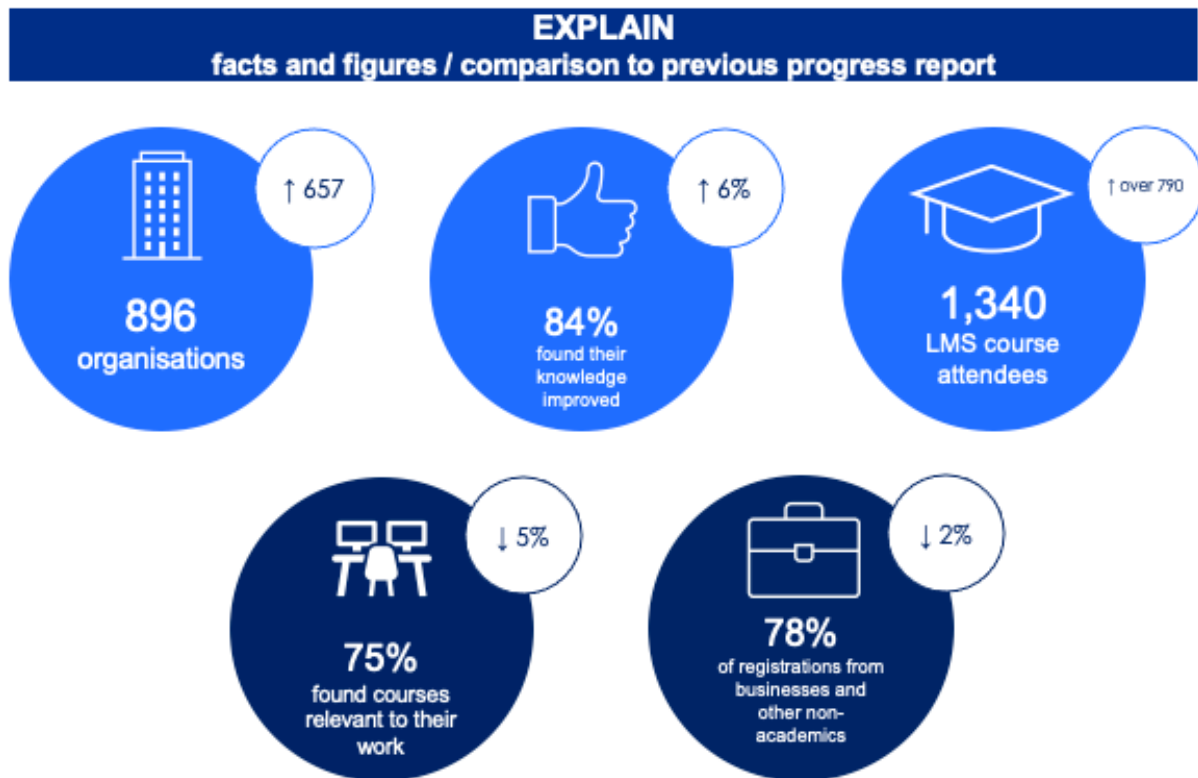
Figure 2   Explain participant feedback on course relevance and satisfaction with the course training

Source: HNCDI monitoring data: Explain post-exit survey. n=114.

The outputs from other workstreams continue to influence the development of new training activities within Explain. For instance, a training course on how to use HNCDI's GeoDN platform for different types of geospatial modelling has been developed. The course is targeted at data scientists and will involve learnings and outputs from the TreesAI project. Similarly, team members from the Emerging Technology workstream are working to produce an introductory training course in quantum computing for Explain. This is in part driven by the higher-than-expected levels of interest in quantum computing.

EXPLAIN
facts and figures / comparison to previous progress report

↑ 657 — 896 organisations

↑ 6% — 84% found their knowledge improved

↑ over 790 — 1,340 LMS course attendees

↓ 5% — 75% found courses relevant to their work

↓ 2% — 78% of registrations from businesses and other non-academics

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

Finally, HNCDI supports 3 strands of activity related to the Hartree Centre's compute capacity.

The procurement of the **on-premise cloud** for the HNCDI programme is complete and is now fully operational. This cloud provision means that HNCDI projects can be developed in such a way that the outputs can be applied across multiple domains. Since coming online, the on-premise cloud has been used across a wide range of Explore and Excelerate projects and will continue to benefit HNCDI projects across the programme's lifecycle and in the future. Use of the on-premise cloud has already resulted in cost savings for the Hartree Centre by migrating from more expensive public cloud resources. The usage of this cloud provision has been steadily increasing and is on-track to reach the target of 70% utilisation.

The **public cloud provision** has been online since the HNCDI programme began and use has steadily increased in line with the project progress of the programme. A new process, designed with greater efficiency in mind, has been launched to secure access to public cloud platforms such as Google and AWS to support the delivery of HCNDI projects. Though the use of the public cloud provision is decreasing as more HNCDI projects are on-boarded to the on-premise cloud platform, the availability of this resource has provided valuable flexibility for the programme to meet the different needs of HNCDI projects and clients.

Construction of the supercomputing centre at Sci-Tech Daresbury began in January 2023 and is on track to complete by summer 2024. In 2023, the HNCDI programme launched and awarded the procurement for the provision of the accelerated HPC systems, with the supercomputer to be installed and available for 2025.

The first system to be installed in the new supercomputing centre will have performance capability of 44 petaflops which means they are capable of running up to 100 trillion calculations per second. This is 20 to 25 times faster than the current platform. As a result, these new supercomputing systems will expand the Hartree Centre's capacity to deliver higher quality, more flexible and secure services to businesses.

Appendix – Interviewees

Area of expertise	Name	Organisation	Role
The Hartree Centre Cardiff Hub	Professor Alun Preece	Cardiff University	Hub Lead
	Luiza Patorski	Cardiff University	Business Liaison Officer
The Hartree Centre North East Hub	Professor Barry Hodgson	Newcastle University	Hub Co-lead
	Dr Ashmita Randhawa	Sunderland Software City	Hub Co-lead
The Hartree Centre Northern Ireland Hub	Dr Justin Quinn	Ulster University	Hub Lead
Emerging Technology	Dr Stefano Mensa	STFC Hartree Centre	Emerging Technology Workstream Lead
HNCDI collaborator	Tim Culmer	Riskaware	Environmental and Geospatial Solutions Capability Lead
HNCDI collaborator	Dr Jan Rogers	Agile Life Sciences	Joint CEO
HNCDI collaborator	Chloe Tregar	Dark Matter Labs (TreesAI)	Research and Analysis