Hartree Centre Highlights 2023-2024



Science and Technology Facilities Council

Hartree Centre

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Note from our Director

Reflecting on my second year as Director at the Hartree Centre, I am proud to see our teams continue to work at the intersection of applied digital research and innovation to deliver exciting digital solutions that make a difference for UK industry.

- Kate Royse, Hartree Centre Director

This year saw the publication of our five-year strategy, setting out our key strategic priorities and how we will work with our partners in the research and innovation ecosystem to place advanced digital technologies into the hands of UK businesses and public sector organisations, regardless of their size. Throughout the year, we have held several stakeholder events to share how this strategy will be realised through our people, partnerships and programmes.

Collaboration is one of our core values, allowing us to connect the dots between technologies, ideas and challenges by providing access to a network of expertise. We formed a strategic partnership with Mersey Care NHS Foundation Trust to pioneer the adoption and integration of advanced digital technologies to optimise patient outcomes. We became part of the new Liverpool City Region Life Sciences Investment Zone, which is uniting the strengths of local business and technology partners to bring even more world-leading innovation and opportunities to the region. We also announced a partnership with PsiQuantum to explore practical industrial applications of quantum computing technologies as part of our commitment to supporting UK businesses to lower barriers to adoption and de-risking investment decisions into emerging technologies. Our agreement with Quantinuum will also expand access to industry-leading quantum computing hardware for businesses and research communities, supporting the roadmap to achieving guantum advantage and realising our role in helping to establish the UK as the go-to place for quantum businesses.

Supporting businesses to unlock the high growth potential of digital technologies is our purpose as the Hartree Centre. We welcomed four early-stage companies this year as part of STFC's Digital Business Incubation Centre. From AI tools to streamline the diagnosis of blood cancers, to developing new supercomputing algorithms that will accelerate digital engineering design processes, we are supporting innovation for societal and economic benefit.

In March 2024, we signed an agreement for the installation of a powerful new supercomputer that will power AI research for industry, and we have been thrilled to see the rapid progress on the construction of our new supercomputing centre over the course of the year which will expand our capacity to support UK businesses.

Our teams continue to demonstrate thought leadership and technical excellence on both the national and international stage, participating in flagship supercomputing, AI and quantum computing conferences and delivering or contributing to over 200 events from training small businesses to convening workshops on exascale computing and the future of compute. The Hartree Centre's continued success can be attributed to our people, who work together to form powerful teams that continuously strive to innovate and create solutions that make a difference for UK society.

Hartree Centre Highlights 2023-2024





Making the future of computing a reality for UK industry

<u>Our new strategy</u> sets out a five-year plan that builds on our achievements to date and continues to deliver significant societal and economic impact for the UK.



Co-created with our staff, collaborators and stakeholders, our strategy sets out our purpose, mission and vision alongside six key strategic priorities that highlight how we will help UK industry to unlock the high-growth potential of advanced digital technologies.



To equip UK industry with the knowledge, skills and compute needed to fully unlock the potential of advanced digital technologies



For UK industry to generate socio-economic growth by exploiting UK compute capabilities to explore and adopt advanced digital technologies

Values

Our values demonstrate and define the way our teams and individuals work as well as how we, the Hartree Centre, work within our communities and behave as part of the UK's research and innovation ecosystem.

Trust

We are proud to operate with integrity and diversity of thought. We are trusted advisors to UK industry.

Collaboration

We use the power of our people, partnerships and networks to unlock the high growth potential of advanced digital technologies for UK industry.

Innovation

We are driven by curiosity; we are not happy with the status quo and continuously strive to innovate by creating solutions that make a difference for UK society.

Knowledge

We can see the bigger picture, connect the dots across technology providers, ideas and challenges. Our people are always open to learning new things and sharing our knowledge to help UK industry explore and adopt advanced digital technologies.



People and Careers

Training UK industry and the public sector to meet the increasing demand for digital skills so that the UK can actively take advantage of the lastest technologies.

Ideas

Exploiting our facilities and expertise to explore and develop transformative technologies and ground-breaking scientific advancements that address national priorities in HPC, AI, quantum and extreme-scale, and cloud computing.

Impact

Creating industrial, societal, and economic impact across the UK by empowering industry to exploit, embed, and adopt the latest advanced digital technologies.

Places

Ensuring the Hartree Centre is recognised as the UK's national facility for providing industry access to worldclass compute resources.

Innovation

Positioning the Hartree Centre as the go-to trusted partner to help UK industry advance understanding and adoption of innovative advanced digital technologies.

Organisation

Operating a modern, sustainable, and effective Hartree Centre that supports the development, safety, and wellbeing of its diverse teams.

Digital innovation for societal and economic impact

The <u>Hartree National Centre for Digital Innovation (HNCDI)</u> is a collaborative five-year programme with IBM which is enabling businesses to acquire the skills, knowledge and technical capability required to adopt advanced digital technologies.

Now in its third year, we have completed the second independent evaluation of the programme, analysing the impact so far across all R&D and training workstreams.

Across our three core R&D focused workstreams, 90 projects were launched and 40 successfully completed. We also engaged with 38 new partner organisations. The projects have started to produce codified knowledge, which was demonstrated in the publication of 43 articles. Under EXPLAIN, our training workstream, we have upskilled 2,033 individuals from 446 organisations with our free courses tailored to industry challenges. The courses received positive responses from participants, with 84% of attendees reporting improved knowledge of digital technologies, and 75% reporting positively about the relevance of the training to their industry sector and challenges.

67%

of companies engaged in R&D projects report an increase in their capacity to innovate as a future benefit

50%

of organisations in EXCELERATE are hoping to reduce their costs because of this intervention

Case Study: <u>Optimising early drug discovery with</u> <u>quantum computing</u>

Early drug discovery is notoriously expensive and time-consuming. Once a drug candidate is identified from thousands of molecules, it must undergo rigorous testing in the laboratory to determine the potential for success as a drug. 90% of clinical trials fail which is an incredibly high failure rate. We worked with IBM using quantum computing techniques to address this.

Our team integrated quantum computing into a classical workflow for drug discovery that used a machine learning algorithm to identify candidates from a database. This boosted the accuracy of selecting an ideal candidate significantly, when compared to classical techniques.

Enhancing drug candidate identification boosts accuracy, cutting both the time and cost of drug discovery by reducing failed trials. This mitigates investment risks for stakeholders and allows resources to be redirected to the most promising drug candidates for further investigation.



Facilitating the growth of a digitally engaged regional SME network

Our Hartree Centre SME Engagement Hubs assist and enable small and medium-sized businesses in regions across the UK to enhance productivity and gain a competitive advantage through the adoption of advanced digital technologies. Through this strategic initiative, we are connecting advanced digital technologies and expertise from the research community and established regional networks of industry-led innovation to the small and medium-sized businesses which make up 99.9% of the UK economy.

The <u>Hartree Centre North East Hub</u> supports SMEs looking towards digital technology, whether that be taking the first steps into learning about data or exploring advanced Internet of Things options, that can be implemented into their organisation. In a collaboration between Sunderland Software City and the National Innovation Centre for Data at

This year, data scientists at the Hartree Centre North East Hub helped local SME Floki Health to <u>develop an interactive</u> <u>visualisation tool, simplifying complex</u> <u>health data for healthcare professionals</u> Newcastle University, the HNCDI programme is leveraging regional support for SMEs to upskill and implement digital solutions.

The <u>Hartree Centre Cardiff Hub</u> empowers SMEs with AI and data analytics in the Cardiff Capital Region and Western Gateway. So far, they have engaged more than 60 organisations and led multiple events to encourage local SMEs to access support for digitisation.

The <u>Hartree Centre Northern Ireland Hub</u>, led by Ulster University, aims to help businesses across the region explore and adopt emerging digital transformation technologies including AI. They have received interest from over 40 SMEs operating regionally across Northern Ireland and are steadily scoping valuable solutions for these businesses to adopt and understand the strategic importance of digital technologies for their organisations.

In a recent highlight, the Hartree Centre Northern Ireland Hub worked with Dublin-based food manufacturer McColgans to <u>optimise their processes</u> <u>and reduce operational costs</u>

The Hartree Centre Cardiff hub has quickly established a 'network of networks', leveraging multiple SME communities and building bespoke solutions

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Making a difference using digital technologies

Our teams work with industry and public sector partners creating solutions that make a difference. From manufacturing to healthcare, our case studies demonstrate our ongoing commitment to creating societal and economic impact across the UK.

Case Study: <u>Developing efficient urban emergency responses</u> with Riskaware

Cities present many challenges for the deployment of an emergency response due to physical obstacles and population density. Riskaware aims to solve this challenge using UrbanAware, a platform that models the release of hazardous materials in urban areas. Due to the complexity of the challenge, it was difficult to identify the most suitable way to use the software and to improve its functionality.

In collaboration with IBM, we leveraged the Geospatial Discovery Network (GeoDN) and the Variational Exploration Module (VEM), which allowed us to run thousands of simulations in parallel and identify the most useful combination of input parameters. UrbanAware's code was also enhanced to run seamlessly across different systems.

Our work optimised UrbanAware's computational performance and enhanced the testing, deployment, scaling and maintenance capabilities of the software, bringing actionable intelligence to our cities sooner.



Image Credit: Unsplash

Case Study: Transforming manufacturing through digital-first design

Vital to UK manufacturing, the glass and steel sectors face a growing challenge to produce materials that are both sustainable and affordable. Funded by Innovate UK, the Com2Coat project adopts the collective expertise of leading partners in key foundation industries to optimise the design process for specialised spray coatings.

Manufacturers use specialised protective coatings to ensure durability but the design process for this is both time-consuming and costly due to the vast chemical combinations and application methods that can be used.

As part of the collaboration, our computational chemistry and materials team developed a workflow capable of simulating the interaction of spray coatings with glass and steel. This helped project partners adopt a digital-first approach, transforming how they designed spray coatings, streamlining timelines and reducing development costs.



Image Credit: Canva

Case Study: Improving patient care and fall prevention with data science

Falls can lead to serious injury among the elderly population. safesteps[™] are a digital healthcare company that create personalised patient care plans based on standardised, comprehensive guidelines. To identify the best interventions for patients, all patient data needs to be processed, standardised and made accessible for GPs and carers through an integrated healthcare dashboard.

We helped to develop a data dashboard to process and standardise data across systems and providers. We also integrated new, standardised classifications to improve fall categorisation, which improves the treatment process for healthcare professionals and patients alike.

This data dashboard is now more accessible than ever and ensures that data gets to the right people at the right time through integration with key NHS internal systems. safesteps[™] are building further on this work through a follow-on project looking at decreasing hospital admissions by reducing fall risk.



Image Credit: Adobe Stock

Maximising industrial impact through our partnerships and programmes

Smart Manufacturing Data Hub

We are working alongside a network of partners in the <u>Smart Manufacturing Data Hub (SMDH)</u> programme to bring data-driven technologies to small- and medium-sized manufacturers across the UK. Through expert guidance, funding and training, we empower manufacturers to boost digital literacy and deliver solutions that support troubleshooting, process optimisation and decision-making, driving productivity.

SMDH offers manufacturers solution packages that are ready-made and free or low-cost, increasing accessibility and maximising impact. Packages provide sensors, software and networks for data collection and upload as well as platform access to monitoring dashboards, which helps SMEs keep track of the industrially relevant metrics including power consumption, carbon emissions and processing conditions.

Our data scientists have developed bespoke analysis pipelines and visualisations through 'Lighthouse projects' under SMDH and our research software engineers have built the Manufacturing Data Exchange Platform (MDEP) which helps manufacturing SMEs gain insights from their data, facilitating decision-making for process optimisation. The platform is live and has already attracted significant industry uptake across the UK.

"It has been great working with SMEs to facilitate their transition towards digital maturity, helping them extract valuable insights from their data to enhance productivity and competitiveness."

 Samuel Omole, Data Scientist, Hartree Centre



Image Credit: SMDH

MDEP Utilisation

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43 datasets shared publicly



>264 datasets shared with limited access

BridgeAl

We are one of four strategic delivery partners in the Innovate UK <u>BridgeAl</u> programme alongside Digital Catapult, the Alan Turing Institute, and the British Standards Institute. BridgeAl is dedicated to driving economic growth and enhancing the UK's competitiveness through the adoption of artificial intelligence (AI) and machine learning. Targeting high-growth sectors such as agriculture, construction, transportation, and creative industries, the programme aims to significantly boost productivity and efficiency.

Over the past year, we awarded 181 BridgeAl Innovation Vouchers, providing businesses with essential technical expertise to facilitate their adoption of AI and its implementation. Additionally, the recent launch of our High Performance Computing (HPC) vouchers has attracted 51 applications, offering businesses access to the advanced computing resources necessary for AI development.

Our training series, Discover Digital Transformation, has also successfully upskilled over 280 individuals. This initiative helps businesses explore and adopt digital, datadriven and AI technologies, ensuring UK industry is prepared for the digital future.

In March 2024, we hosted a BridgeAI transportation workshop, attended by 55 participants from across the transport and automotive sector. It featured a panel of technology and industry experts who discussed the application of AI for transport. The discussions highlighted how AI can be leveraged to increase productivity, foster innovation, and develop new solutions tailored to sector-specific needs. A total of **£2,210,000**

awarded to UK businesses through innovation vouchers





of companies surveyed said they were satisfied with the support provided by the Hartree Centre through BridgeAI



Successful BridgeAl Innovation Voucher applications by sector



BridgeAI Case Study: <u>Finding cheaper and more sustainable</u> ceramic glazes using data science

In the ceramics industry, choosing the right glaze is not only about aesthetics but also economics and sustainability. Through the Innovate UK BridgeAI programme, ceramics company Box O Fun accessed our data science expertise to develop a search function that helps ceramicists easily find cost-effective and sustainable glaze recipes that offer the desired glaze properties.

Using automation, our data science team collated data on 25,000 glazes. This was used to build the glaze search function that allows users to input available materials and their quantities to find economical recipes without compromising on glaze properties.

The newly developed tool helps ceramicists find glazes that can be made from cost-efficient and available materials, including leftover materials. This offers Box O Fun increased resilience against supply chain and economical challenges while also driving environmental sustainability by reducing waste.



Image Credit: Box O Fun

Fusion Computing Lab

Making energy a commercial reality with supercomputers and AI

Our collaboration with the UK Atomic Energy Authority (UKAEA) leverages cutting-edge supercomputing and data science techniques to advance fusion technologies, paving the way for a low-carbon future. Our expertise in supercomputing and AI, combined with UKAEA's knowledge of fusion will accelerate digital-first design solutions that will reduce the need for costly, time-intensive real-world prototyping. We will achieve this by developing digital twins of fusion devices, where we will enable scientists and engineers to test viable power plant technologies virtually. This partnership is also fostering the growth of a new industrial sector, involving pioneering SMEs, universities, and engineering giants poised to deliver and commercialise fusion.

"Our unique relationship with Hartree Centre is combining UKAEA's heritage in delivering world-class fusion science with STFC's experience in supercomputing, big data, and artificial intelligence. By tapping into Hartree Centre's experience in engaging industry, we aim to democratise the tools we are designing and the skills and knowledge we are developing across the UK's rapidly growing fusion supply chain. Our mission is to ensure that the fusion sector is 'digitally adept' in leveraging the disruptive power of extreme scale computing and AI, creating a paradigm shift in the way fusion powerplants will be certified, regulated, and operated for promoting a 'simulation first' approach to engineering design."

 Rob Akers, Director of Computing Programmes & Senior Fellow, UK Atomic Energy Authority.

Developing skills through industry-focused training

Our training and skills development this year has accelerated knowledge and improved understanding in advanced digital technologies like AI, HPC and quantum. Our training team works collaboratively across a variety of programmes to upskill our industry partners and raise the profile of skills requirements for both public and private sector organisations.

Our training and skills offering is always in line with cutting-edge developments across industry and academia and is embedded throughout our programmes and strategic collaborations, allowing us to look forwards to the future of emerging digital technologies and guide UK businesses along the way. Under our HNCDI programme we continue to work for industry, utilising our SME Hubs networks to promote and advance the skills of SMEs across the UK. Our training portal and learning pathways are free tools used by organisations to understand how to apply digital technologies and explore new concepts.

We offer a comprehensive range of <u>training</u> <u>opportunities</u>, including self-paced courses, online and in-person workshops, programming schools, and personalised one-to-one mentoring, to provide tailored solutions that best meet your training needs. Recently, we collaborated with Unilever to develop a mentorship program specifically designed to support a member of their data science team.

Case Study: Kick-starting careers with personalised mentoring

With Unilever's growing cohort of new data science practitioners, the company approached the Hartree Centre to provide personalised

one-on-one mentoring for a new team member, supporting their development as a data science apprentice.

Having worked closely with Unilever over the past ten years, we are well-equipped to support their request. Over six months, our team designed and delivered a tailored development programme for the apprentice, providing bespoke one-onone mentoring through weekly sessions.

To enhance the apprentice's coding skills and expand their practical machine learning knowledge, our team supported them in designing and creating a fully implemented data dashboard for 2,033 users to facilitate global sharing of internal resources. This bespoke training has expanded the apprentice's skillset, which they have in turn shared with their team at Unilever, further boosting their confidence and expertise. 2,033 people

attended training courses from AI to HPC and Quantum

446 organisations

upskilled in digital technologies

"The Hartree Centre's knowledge and teaching has allowed me to grow as a data scientist and helped me deliver key data insights back to my team. Their ability to explain complex topics has been invaluable in developing my data skills."

Ryan Brocklebank,
Data Science Apprentice, Unilever

Conferences and events

Expanding our national and international profile

In 2024 we continued to grow our international profile, sharing our expertise in advanced digital technologies by participating in a series of industry events and delivering technical workshops.

We have a long history of attending leading international conferences like Supercomputing and the International Supercomputing Conference, fostering collaboration and sharing our research and innovation insights in HPC, AI, quantum, extreme-scale and cloud computing.

Over the last year we have organised a series of industry-specific events spanning from the automotive sector to healthcare, helping to empower organisations to explore and adopt cutting-edge technologies. For the second year running, we hosted an 'On the Trail to Exascale' workshop. This brought together over 50 industry and academic representatives from leading UK and international organisations to discuss how emerging technologies can address global challenges from decarbonising the economy to accelerating drug discovery. In collaboration with the Smart Manufacturing Data Hub programme, we hosted a digital transformation workshop to share industry solutions and funding advice, helping manufacturers looking to modernise their operations with automation and data analytics. We also hosted a quantum discovery day event for the healthcare industry to help businesses and the public sector explore how quantum technologies can help tackle sector challenges and drive innovation.

Our industry engagement specialists have an active presence in the digital innovation community, gaining an insight into the challenges that UK businesses face across multiple sectors. Our teams attend leading events including the Institution of Mechanical Engineers International EV Batteries conference and the Society of Motor Manufacturers and Traders (SMMT) International Automotive Summit. With our presence at UK and internationally renowned events, we demonstrate our thought leadership in emerging technologies, establishing ourselves as a trusted partner in these fields.





Our people

The Hartree Centre has continued to grow over the last year. As of July 2024 we had 117 scientists and technologists researching and developing solutions to challenges around digital technologies, supported by 70 professionals dedicated to managing, communicating, training and providing access to the Hartree Centre infrastructure and expertise. Continuing our growth infuses the centre with the fresh ideas, talent and knowledge that allows us to see the bigger picture and make a difference for UK society.

We value all our people and want to see them grow and flourish at the Hartree Centre. To make this happen, we provide learning opportunities for our staff to pursue relevant skills and projects that inspire them. Currently we have 4 team members completing upskilling apprenticeships, and we are supporting 6 early career apprenticeships.

"Working at the Hartree Centre has allowed me to pursue several different career development opportunities like working towards a Senior Leader apprenticeship which led to me completing an MBA and I'm currently working on a continuous improvement project with associated Yellow Belt training. Collectively, these opportunities have helped to improve our project management processes across the centre, allowing my teams to support and collaborate with other teams and our project partners more effectively."

- Gemma Curtis, Portfolio and Programme Manager



"The Hartree Centre has provided me with invaluable opportunities to manage and serve as a technical lead across a range of projects. This hands-on experience has allowed me to apply my knowledge and skills in real-world scenarios, significantly enhancing my professional development. Working alongside talented colleagues has also afforded me the chance to receive mentorship from and engage in problem solving with industry experts. The insights and guidance from these experienced professionals have not only enriched my technical abilities but also fostered a deeper understanding of strategic decision-making and leadership skills, empowering me to grow both personally and professionally."

- Emre Sahin, Quantum Software Engineer

We also know the importance of connecting and engaging our colleagues through community. To facilitate healthy networking and to allow our colleagues to get to know each other, this year we have held several team building events which have received excellent feedback from our staff. We will be hosting more events like these next year to continue fostering a healthy professional community for our colleagues.





