



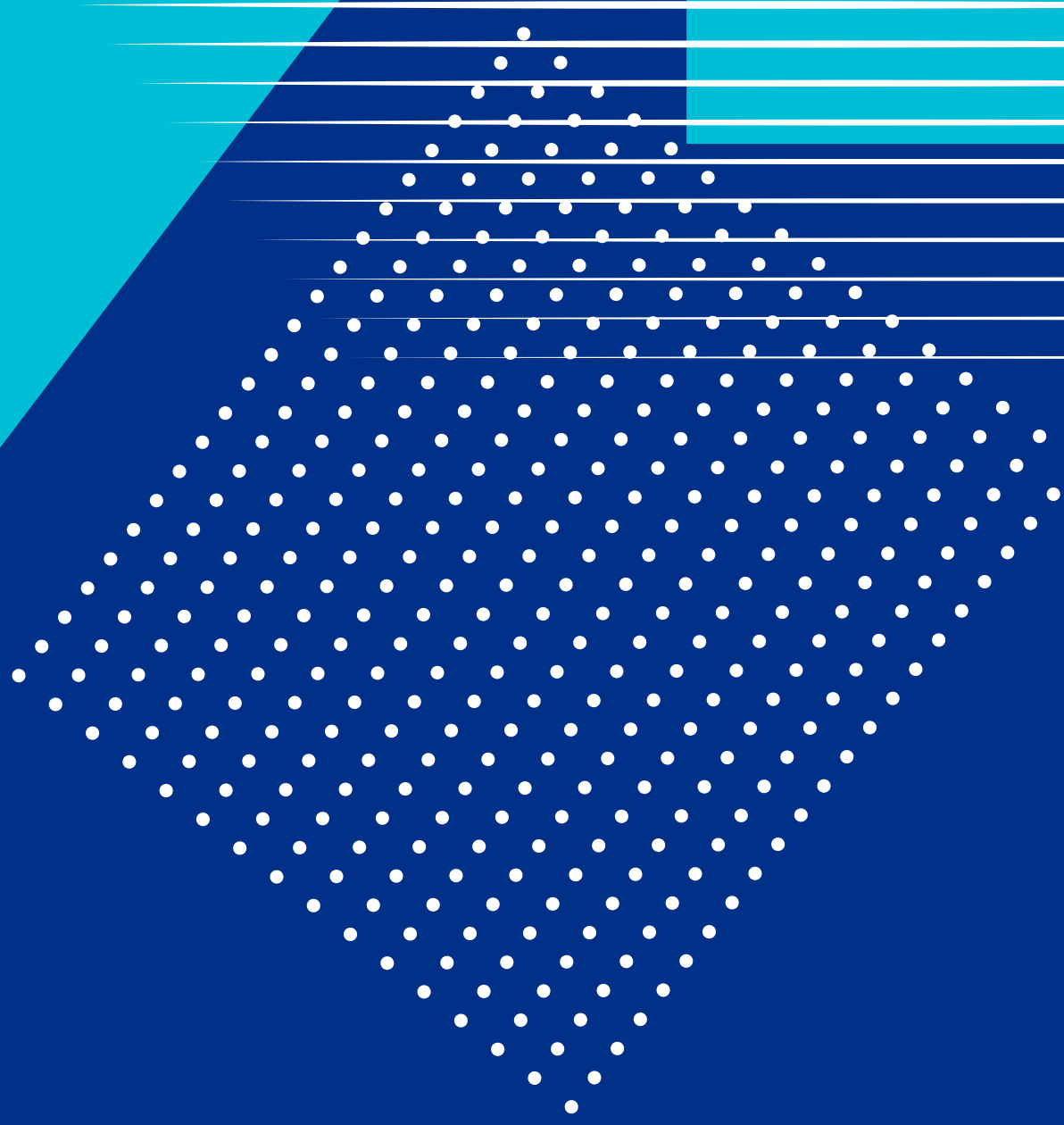
Science and
Technology
Facilities Council

Hartree Centre



Hartree Centre

Highlights 2022-2023



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Note from our Director

After completing my first year as Director here at the Hartree Centre, I have seen first-hand the huge impact our work makes in supporting UK industry to embrace and adopt advanced digital technologies.

As a centre, we pride ourselves on the strength of our collaborations. One real highlight has been our work with the US National Laboratories, where we are developing an exascale-ready modelling and simulation environment for nuclear fusion powerplants. This will also augment our collaboration with the UK Atomic Energy Authority (UKAEA), where we are helping to deliver the UK Government's Net Zero goals by accelerating the vital mission of developing sustainable fusion energy and de-risking the adoption of pre-exascale and exascale computing for UK industry.

To keep pace with our rapidly evolving digital landscape, innovation is the key to success and as we reflect on the accomplishments of the past year, it is evident that we have played a pivotal role in delivering societal and economic impact. I was especially pleased to see our work mentioned in several government white papers this year, most notably the *Independent Review of the Future of Compute*. We will expand upon our significant achievements, partnerships and initiatives undertaken further throughout this highlights document.

The Hartree Centre has forged strategic partnerships with industry leaders such as IBM, Atos and Unilever as well as academic collaborations with the University of Liverpool and Manchester. These collaborations have enabled us to tap into a wealth of expertise and resource, fostering an ethos of co-design and knowledge exchange. This year we have expanded our reach across the UK by establishing regional SME engagement hubs in Northern Ireland, North East England and Cardiff, providing enhanced accessibility to digital technologies for small and medium-sized enterprises.



Kate Royle, Hartree Centre Director

Digital innovation has the power to revolutionise multiple industries and create solutions that have a positive impact on society. From the various sectors and technology domains we work in, of particular note this year is our work on accelerating drug discovery with AI, enhancing climate resilience through digital twins and the use of quantum computing for transport and logistics.

As digital technologies continue to evolve, there is a growing need for skilled professionals who can harness their potential. At the Hartree Centre, we recognise the importance of training and education in equipping individuals with the necessary skills to thrive in the digital age and we will outline how we have been working to expand our training portfolio to upskill the UK workforce.

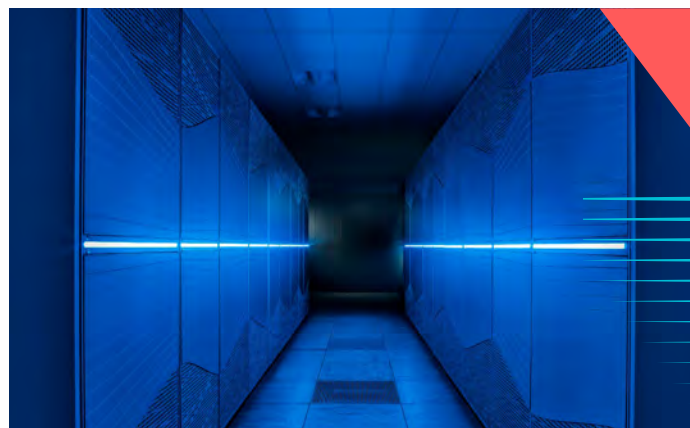
Finally, the success of the Hartree Centre can be attributed to our dedicated and talented team. Comprising of experts from diverse backgrounds, including technologists, researchers and professional services colleagues, our teams combine a wealth of knowledge and experience to drive digital innovation. Their passion for pushing the boundaries of what is possible is evident in the impactful solutions and collaborations they have facilitated.

Our technologies

Exploiting the opportunities presented by high-performance computing, data science and artificial intelligence (AI) technologies is the key to faster innovation, more confident decision making, sustainable operations and increased competitive advantage.

These technologies are continuing to transform the innovation landscape, using the speed of supercomputers, state of the art data analysis and visualisation to revolutionise traditional R&D methods to reduce costs while increasing accuracy and productivity.

We are making the power of advanced digital technologies accessible to industry – lowering the barriers to their use and focusing on market-led research, innovation and development challenges to support business and economic growth.



Scafell Pike

Systems and Platforms

Scafell Pike

- Tightly coupled Intel and Nvidia architectures
- Includes 24,960 Intel Skylake cores
- Integrated DDN Exascaler storage appliance
- Mellanox InfiniBand interconnect
- Direct liquid-cooled compute nodes

Secure Data Facility

- Openstack and Ceph for medium-term storage of project data with some capacity for analysis/query

Cloud Facilities – On-Premise

- RedHat OpenShift (self-service)
- OpenStack VM provisioned
- AMD CPU/GPU, Nvidia A100, Alveo U200

Cloud Facilities – Public Cloud

- Contracts with all major cloud providers
- Enabling rapid operationalising of workflows
- 24/7 uptime

Quantum Computing

- Quantum software development service comprising two Atos Quantum Learning Machines, each capable of simulating up to 38 quantum bits (qubits)
- IBM Q access

Energy Efficient Data Centre

- Construction of our new Supercomputing Centre is underway, and work is expected to be completed in 2025

Visual Computing Suite

- Immersive visual computing labs based onsite at the Hartree Centre connected to our compute and data facilities

JADE

- Operation of EPSRC Tier-2 national service
- Tightly-coupled Nvidia Tesla V100 (504 total GPU count)

Digital innovation for societal and economic impact

Digital innovation has the power to transform several industries and drive growth by improving performance and productivity, creating solutions that make the world a better place.

From accelerating drug discovery using artificial intelligence (AI) to creating digital twins for climate resilience and using quantum technology to solve transport and logistics challenges, at the Hartree Centre, we are committed to supporting the UK ambitions of being a global science and technology superpower

We help UK businesses and organisations of any size to explore and use supercomputing, data analytics and AI technologies for enhanced productivity, smarter innovation and economic growth. Established in 2012 to increase the adoption of digital technologies across UK industry and solve R&D challenges, we are backed by significant UK government funding and proud of our strategic partnerships with industry leaders such as IBM, Atos and the University of Liverpool. We are based at Sci-Tech Daresbury in the Liverpool City Region with 150 staff based across 3 STFC campus locations in the UK. This year, we also launched our regional SME engagement hubs in Northern Ireland, North East England and Cardiff.

Hosting some of the most advanced digital technologies and experts in the UK we collaborate with industry and the research community to explore the latest technologies, upskill teams, and apply practical digital solutions to individual and industry-wide challenges for societal and economic benefit. We are committed to making an impact on UK industry; delivering value and creating benefits that matter is at the heart of everything we do. The next evaluation of our major programme, the Hartree National Centre for Digital Innovation, is due to be published in 2026.

The Hartree Centre is part of the Science and Technology Facilities Council (STFC) – one of Europe's largest multi-disciplinary scientific research organisations – within UK Research and Innovation (UKRI), building on a wealth of established scientific heritage and network of international expertise to help the UK stay at the forefront of pioneering computational science and digital innovation.



Powering an innovation-led economy

Hartree National Centre for Digital Innovation. Enabling UK businesses and the public sector to explore and adopt digital technologies including AI and quantum computing for productivity, innovation and economic growth.

The Hartree National Centre for Digital Innovation (HNCDI) is our 5-year collaborative programme with IBM Research that offers a safe and supportive environment for organisations to explore the latest digital technologies and skills, develop proofs-of-concept and create roadmaps to apply them to industry and public sector challenges effectively. Driven by industry requirements, HNCDI helps individuals and organisations with an appetite for change who are ready to innovate by creating useful solutions, enhancing and adapting products and processes, adopting new digital technologies and expanding into new markets.

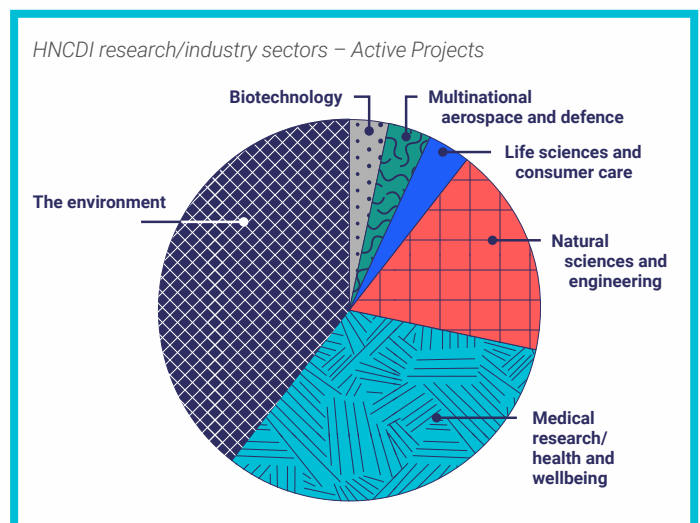
In November 2022, we hosted a Digital Innovation for Economic Resilience event at IBM London, showcasing pioneering digital innovation stories that were brought to life through case studies and demos. The expertise demonstrated by the Hartree National Centre for Digital Innovation attracted over 70 delegates from UK industry and Government keen to learn how we are using advanced supercomputing, data analytics and artificial intelligence to achieve productivity and sustainability goals.

In May 2023, the Technopolis Group completed the first evaluation of HNCDI, covering the key activities and highlights from the first 18 months of the programme.



HNCDI Digital Innovation for Economic Resilience and Productivity event speakers, left to right: Mark Thomson (STFC), Sreeram Visvanathan (IBM), Kate Royse (STFC Hartree Centre), Peter Waggett (IBM Research) and David Bunton (Reprocell). November 2022

As of May 2023, HNCDI has a total of 66 projects across three research and development workstreams: Explore, Emerging Technology and Excelerate. 28 projects are ongoing, 30 have closed and 8 are ready to begin. The projects within HNCDI cover a variety of industry sectors outlined below, demonstrating the breadth the programme has achieved during two years of operation.



23* projects received approximately

£321,760

in voluntary effort and software from 15 organisations

65

new STFC and IBM team members

* from July '21 to Dec '22

21

research publications for 14 HNCDI projects, each publication cited twice

Case studies:

NSG Pilkington embrace data science

NSG Pilkington manufactures and processes glass for the architectural and automotive sectors. Collaborating with the Hartree Centre on two materials discovery projects within HNCDI inspired a company-wide recognition of the potential business applications related to data science.

NSG piloted a programme to train their staff in data science through the HNCDI EXPLAIN training programme, recognising the Hartree Centre as a reputable and trusted source working at the cutting edge of digital technologies. The company was drawn to the flexible course delivery and range of experience levels.

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

Using AI to map the risk of flooding

Mapping the risk of climate events requires the collection of comprehensive datasets that are typically analysed through a time-consuming and semi-manual process. Through HNCDI EXPLORE, we developed a machine learning algorithm to identify past and current flood events using satellite data.

Our team trained the algorithm using suitable open-access ground-truth data, verifying this capability against a set of known flood events. Applying AI accelerated the process of identifying and labelling flood event data, which was then fed into a suite of related modules all hosted on cloud platform developed under HNCDI called the Geospatial Discovery Network (GeoDN).

This platform can map multiple climate events and seeks to improve the resilience of UK infrastructure, enhance our capability to address damage and prepare crisis responses across multiple climate applications.

A brand-new supercomputing facility in the North West

In 2023 construction began on a new £42 million supercomputing centre at Daresbury Laboratory and procurement is currently underway for new, more powerful, supercomputing systems to support our rapidly expanding supercomputing and AI activities.

Expected to be completed in 2025, this will expand our capacity to support UK industry and deliver an even better quality, more flexible and secure service to businesses.

We anticipate that the first system to be installed in our new building will have a performance capability of between 80 and 100 petaflops (up to 100 trillion calculations per second), making our new system 20 to 25 times faster than our current platforms.



Groundbreaking ceremony to celebrate construction of the new Supercomputing Centre at Daresbury Laboratory, February 2023

Launching a UK digital innovation network for SMEs

This year, we awarded £1.5 million each to Cardiff University, Newcastle University and Ulster University to fund small and medium-sized enterprise (SME) engagement hubs for three years as part of the Hartree National Centre for Digital Innovation (HNCDI). The Hartree Centre SME hubs will enable regional small businesses across the UK to gain a competitive advantage through the adoption of advanced digital technologies including data science and AI.

Each hub will use their own in-house expertise, local sector knowledge and industry engagement experience to provide targeted support for regional SMEs to enhance competitiveness and growth through the adoption of digital technologies and methods.



Hartree Centre SME Engagement Hubs launch event at Cardiff University, June 2023

“

We look forward to working with the Hartree Centre to grow capacity and capability in our regional digital transformation ecosystem, enabling inclusive and responsible innovation across the SME community.”



Professor Alun Preece, Hartree Centre | Cardiff Hub



Hartree Centre | Northern Ireland Hub
delivered by Ulster University and Cambium LLP



Hartree Centre | North East Hub
delivered by Newcastle University and Sunderland Software City



Hartree Centre | Cardiff Hub
delivered by Cardiff University

Digital technologies that make a difference

A digital-first approach to valve design for hydrogen and carbon capture

We are working with Oliver Hydcovalves – suppliers and manufacturers of high-performance pipeline ball valves for hydrogen transport – to accelerate valve design and testing using supercomputers.

Our Software Engineers developed a Finite Element Analysis (FEA) solver capable of calculating displacements and stresses inside a valve and then generated accurate computer simulation meshes that were run on our supercomputing facilities.

These visualisations offered detailed models of stress and displacement in valve assembly and provided valuable insight for the design team to analyse the state of valves when under pressure.

The power of fast, high-quality simulations coupled with the FEA solver helped Oliver Hydcovalves test highly detailed operating parameters, generating a much wider set of results than would be feasible to do with solely physical testing. As a result of the collaboration, the amount of prototyping and testing needed was decreased, reducing costs while optimising the process and helping the business to address further hydrogen and carbon capture challenges.

“

The Hartree Centre has allowed us to use specialist techniques to refine our designs to a level that otherwise would have been beyond our reach.”

Nick Howard, Oliver Hydcovalves

Image credit: Adobe Stock



MATERIALS

Accelerating materials discovery

Computational materials discovery involves searching vast material spaces for potential candidates that have the optimal combination of suitable properties for target applications. High fidelity predictions are required to make meaningful calculations, so navigating a material space containing tens or hundreds of thousands of materials presents a significant challenge.

Our Materials Discovery Engine (Hartree-MaDE) is a tool that simplifies and automates the process of materials discovery. With a main focus on alloys, the tool can still model all hard materials that exhibit crystalline order, including solid ordered phases of polymers.

Hartree-MaDe only needs users to add the structure and composition of component materials, it then automatically builds a database of every possible substitutional alloy that can be engineered from combinations of the base materials, allowing users to go forward and quickly identify the best candidate materials for their target application.

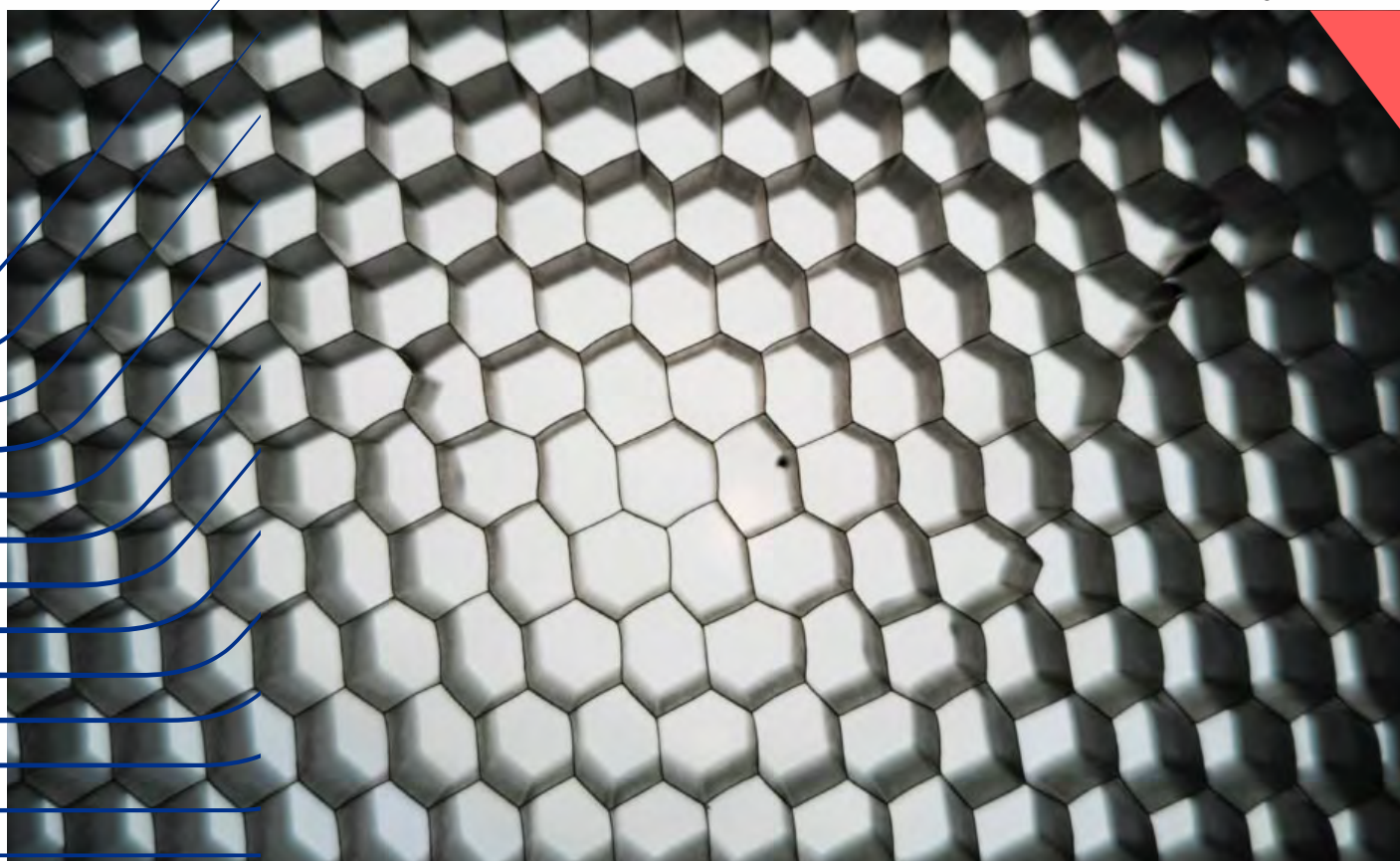
This de-risks and accelerates materials discovery while significantly reducing development costs at the same time. Businesses can use the tool to supply them with candidate materials without the need for expensive trial and error procedures in the lab. It can also help to identify new materials by predicting a range of thermal and mechanical properties, accelerating materials discovery for UK industry.

“

Working with The Hartree Centre enabled us to efficiently explore an extremely complex area of ceramic material discovery for a niche application where currently available options are far from ideal.”

Richard White, Lucideon

Image credit: Pexels



HEALTH AND SOCIAL CARE

Building a data-driven gaming dashboard to support autistic children

We are working with game studio Autsera to develop an in-game dashboard that gives parents and teachers a clearer picture of their children's progress while also identifying areas where extra support is required.

Autsera helps autistic children to communicate and interact socially by creating educational gaming apps centred around fun and engaging science-based gameplay. EmoGami is an app that asks children to match emotions with facial expressions through more than 800 puzzles, spread across 10 levels of increasing difficulty.

To help understand a child's performance as they progress through the app, Autsera were looking for a way to quantify and track a child's journey and present this information to parents, carers and teachers in an accessible, digestible format.

Our data science team carried out a statistical analysis of anonymised data from app users, using this to create a revised scoring matrix that captures variations in game performance over time, allowing results from different puzzles within the app to be compared. The team went on to produce a dashboard to illustrate the new scoring metrics, using simple charts to show a child's progress over time and highlight emotions they were able to successfully match to facial expressions.

“

Thanks to the new scoring matrix, we can show steady, less volatile and more representative data of a child's progress over time in EmoGami. The calculations make more sense, making the monitoring module more reliable and EmoGami more trustworthy.”

Inas Ismail, Autsera

Image credit: Adobe Stock



ENVIRONMENT

Digital twinning for climate resilience and public safety

From medical equipment going offline to an emergency service call operator losing contact, disruption to public services during extreme weather can be devastating.

In the Climate Resilience Demonstrator (CReDo), we are using connected data and virtual modelling to investigate and enhance the reliability of energy, telecoms and utilities services under extreme weather conditions.

Digital twins can help organisations make better decisions by providing access to the right information at the right time, which could be the key to keeping people safe through more resilient infrastructure. We are providing data engineering leadership and expertise to the CReDo consortium.

The resulting digital twin proof-of concept demonstrates how infrastructure operators can use secure, resilient information sharing across sector boundaries to mitigate the effect of flooding on essential service delivery and performance. Alongside the potential to reduce disruption and ensure public safety, CReDo shows how energy, telecoms and utilities operators could also benefit from connected digital twins by reducing the cost and time taken to resolve extreme weather disruption.

“

Trying to predict and mitigate the effects of climate change when you can only see a small part of the bigger picture is almost impossible. Connected data is the key.”

Ben Mawdsley

Image credit: Pexels



Digital innovation through collaboration

Smart Manufacturing Data Hub

We're supporting small and medium-sized manufacturers across the UK to become more competitive and productive through the power of data-driven technologies. Alongside a network of partners, ... we provide expert training and guidance, develop digital solutions, allow companies to explore and evaluate their existing processes, make productivity improvements and operational cost savings, de-risk investments and help businesses enhance their digital maturity and unlock new insights from their data. Our team are developing the SMDH Virtual Hub, a cloud-hosted compute platform for the secure analysis of SME manufacturing data.

**MADE
SMARTER**
INNOVATION

SMART
MANUFACTURING
DATA HUB

BridgeAI

This new £100 million Innovate UK-funded programme aims to drive growth and competitiveness in the UK economy through the adoption of artificial intelligence (AI) and machine learning. Focusing on businesses in sectors with high growth potential such as agriculture, construction, transportation, and creative industries, the programme aims to enhance productivity and efficiency through AI.

Businesses can access expert support from the Hartree Centre with £5000 or £15,000 innovation vouchers that can be used to explore the benefits of integrating AI into their operations. Our Hartree Centre Training Portal also helps businesses get to grips with AI, modelling and data science through a variety of self-paced, virtual courses and live sessions open to all businesses to access at a time that suits them.

Partners:

- Innovate UK
- Digital Catapult
- Alan Turing Institute
- KTN
- BSI

A live demonstration of an SME project



Delivering regional impact

We were delivery partners in two European Regional Development Funded programmes that each ended in 2023.

C&W4.0

November 2020 – September 2023

The Hartree Centre worked with 14 SMEs under the C&W4.0 programme, offering fully funded support for manufacturing SMEs across Cheshire & Warrington to accelerate opportunities for growth and investment using digital technology.

It enabled businesses across the region to develop smarter processes and products, solve problems and stay ahead of the competition by adopting new technologies emerging from the fourth industrial revolution (Industry 4.0).

Partners:

- Virtual Engineering Centre (University of Liverpool)
- Liverpool John Moores University
- The Northern Automotive Alliance

LCR4 START

April 2020 – March 2023

At the Hartree Centre we also worked with 12 SMEs under the LCR4 START programme, supporting SMEs and supply chains in the Liverpool City Region to discover and adopt digital technologies for a competitive advantage.

It helped companies to innovate, digitise and improve their processes through short projects that offered technical and business support to create digital roadmaps and explore new technologies.

Partners:

- Virtual Engineering Centre (University of Liverpool)
- Liverpool John Moores University
- Sensor City
- Growth Platform
- University of Liverpool

Demonstration of the Hartree Centre's Virtual Wind Tunnel

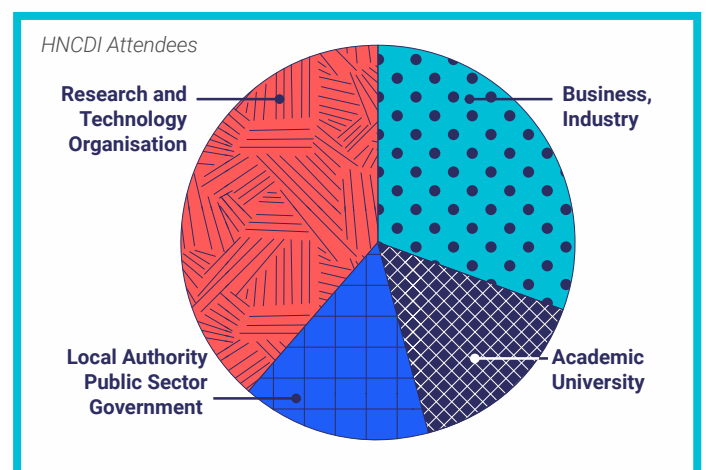


Application focused training and education in digital technologies

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

We run a range of hands-on training courses, webinars, workshops and events each year that open up the potential of digital technologies to new audiences, upskill UK industry and train the next generation of digital experts.

Our courses are flexible, delivered online or in person and often in collaboration with our globally recognised partners like NVIDIA, IBM and Atos. You might choose our self-learning modules to learn at your own pace anytime, anywhere or join a live event where you can meet our team of experts that will help you get to grips with the latest tools and techniques.



Creating tomorrow's technologists

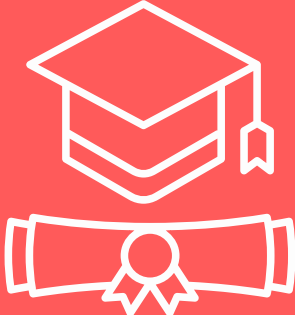
We offer a range of postgraduate training opportunities through Centres for Doctoral Training and MSc programmes.

We use our track record with UK businesses to ensure that projects undertaken by the CDTs have real industry challenges built in, cultivating industry-relevant and cutting-edge technical skills for the next generation of computational science, data and AI experts.

Nandini is part of the AI team at the Hartree Centre and is also a PhD student at the University of Liverpool. Her research is focused on using machine learning methods for omics data, with a specialisation in graph techniques, exploring the intersection of two disciplines – biology, and computer science.

Our team currently provide support and supervision to

20
PhD
students




An interactive training session for PhD students.

“

The Hartree Centre has been a great place to start my career because I can get involved in work that diverges from traditional machine learning such as network based distributed methods, software engineering and biological data interpretation. I feel like I have a perspective on and the opportunity to contribute to real-world projects in industry, alongside the flexibility of academic research. The development of techniques to enhance precision medicine and targeted drug discovery is a particularly accelerated field after the Covid-19 pandemic, and it is exciting to apply my skills and be part of that.”



Nandini Gadhia, AI Researcher

Our people

The Hartree Centre is named after Douglas Rayner Hartree, a mathematician, physicist and champion of early electronic computer development. His passion for innovation and technological advancement makes him an ideal representative for what we do at the Hartree Centre today.

Our expertise covers a diverse set of disciplines. All staff at the Hartree Centre are working to translate the latest computational advances into digital solutions that deliver an effective and sustainable economic impact for UK businesses. The skills and knowledge that staff possess range from chemistry, physics, mathematics, software engineering, data science, technical architecture, and visualisation engineering to system administration, project management, communication, evaluation and business development.

The Hartree Centre continues to grow, now with over 150 staff working as part of our team. 98 are considered as researchers and technologists with over 40 more engaged in supporting the centre to fully achieve its strategic vision.

We are dedicated to the continuous training and development of our people. We have 10 people currently engaged in upskilling apprenticeships and a further 8 apprentices that are new to the centre. Our staff training and development ranges from Level 3 (equivalent to two A Levels) to Level 7 (equivalent to Master's degree) and takes place across a variety of disciplines which is reflective of our broad skillset.

- Professional Services
- Data Science
- High Performance Software Engineering
- Research Software Engineering

“

I joined the centre over six months ago and I found the whole process very enjoyable and a big confidence boost. During the application process, my skills and experience were recognised and embedded into my current workplan. It feels so wonderful to be working in a centre that recognises what you can bring to the team from the outset.”

Hayley King



“

We can do really important work here because of the flexibility and the collaboration we have between the different departments of our centre, we are able to pull expertise from one specific field to take what is useful and apply it to different sectors and industries.”

Francesca Schiavello



“ I am a High Performance Software Engineer who has just completed my Level 7 Apprenticeship. I come from a background in Software Development but I'd always missed working in science and research from my time at university, so the opportunity to come back into that kind of collaborative environment, was something that really drew me to the Hartree Centre and it's one of the reasons I love working here. I like learning as much as possible and there are so many interesting people here which means I come away every day thinking I've learned so many new, exciting things from those around me.”

Victoria Atkinson



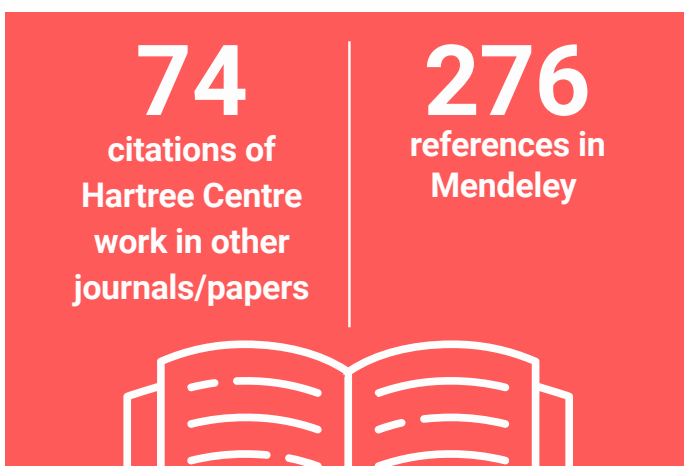
Supporting the UK to become a global science superpower

In 2023, we were featured in several UK Government publications including the Department of Science, Innovation and Technology's (DSIT) [National Quantum Strategy](#) and [Future of Compute Review](#).

A significant number of our success stories and case studies were used to demonstrate the potential of emerging digital technologies to enhance productivity and innovation in UK industry. One such case study – our collaborative AI flood detection work with IBM, funded through HNCDI – was also featured in the Geospatial Commission's [UK Geospatial Strategy 2030](#).

As a key player in the field of advanced computing research and innovation, we're thrilled to be working to ensure the UK has the skills and infrastructure to take a global lead in game-changing digital solutions.

Our team of 150+ Hartree Centre staff collaborate with national and international research communities to push the boundaries of applied emerging technologies. Of these team members, 98 regularly engage in publishing their research findings, with **34 journal articles** published from May 2022 – May 2023.



Uniting supercomputing innovation across Europe

The UK was represented in the EuroCC programme by the STFC Hartree Centre in collaboration with Edinburgh Parallel Computing Centre (EPCC) at the University of Edinburgh.

The initial two-year programme, which concluded in 2022, coordinated high performance computing (HPC) research and innovation activities across Europe, providing unified routes into HPC research and development capabilities for industry, academia and the general public in 33 participating European countries.

The EuroCC network enabled closer international collaboration and knowledge-sharing between supercomputing research centres, boosting efficiency and helping to establish best practice for industry engagement and training practices across the continent.

EuroCC was funded jointly by the European Commission and national funding programs in the partner countries.



The Hartree Centre team representing the UK at the EuroCC conference 2022 in Montenegro

International Association of Supercomputing Centres

We are proud to be founding members of a global effort to bring together public computing centres alongside:

- Lawrence Livermore National Laboratory (LLNL), California, USA
- National Center for Supercomputing Applications (NCSA), Illinois, USA
- Leibniz Supercomputing Centre (LRZ), Germany, Europe

With key strategic goals including solution-finding for common challenges, fostering communication and collaboration among other centres and users and sharing best practice for centre management.

Strengthening UK-US collaboration

We are working with the US National Laboratories - Oak Ridge National Laboratory and Lawrence Livermore National Laboratory – and the UK Atomic Energy Authority via the US Exascale Computing project to test and develop an exascale ready modelling and simulation environment capable of delivering for delivering rapid, advanced prototyping of nuclear fusion powerplants. This will help to achieve UK Government Net Zero goals through the delivery of commercial fusion power and will de-risk the adoption of pre-exascale and exascale computing in the UK, placing us in a strong position to build world-class computing capabilities.

“

Worldwide, there's over 100 publicly funded supercomputing centres which exist to serve a user community for public benefit, and we want to bring people together to talk about common challenges and best practice.”

Wayne Miller, Lawrence Livermore National Laboratory



Driving future investment decisions into emerging technologies

In June 2023, we hosted 'On the Trail to Exascale', a workshop bringing together 50 representatives from UK and international industry, academia and public sector organisations.

We gathered to discuss how emerging technologies can address global challenges such as clean energy and decarbonising the economy as well as accelerating materials and drug discovery.

With visitors from the Department for Science, Innovation and Technology (DSIT), UK supercomputing centres and US representatives from Lawrence Livermore National Laboratory (LLNL) and Oak Ridge National Laboratory (ORNL), we had 2 days of lively discussion looking at how to make exascale technologies more accessible. This engagement will encourage industry adoption with new collaborations and plans to diversify the workforce of tomorrow.



Exascale

“Until now, there have been many problems which have been impossible or extremely difficult to solve, as they require high-precision simulation of complex systems or the intensive use of artificial intelligence (AI) to analyse large datasets. Exascale computing can be used to model this kind of complex problem, from pandemics and climate resilience to simulating new forms of energy production such as fusion. It can also be used for materials development and drug discovery – the applications are endless. The Hartree Centre is set to play a key role in the UK journey to become exascale ready, and I for one, am excited to be part of the exascale revolution.”



Kate Royse, Hartree Centre Director

Case study:

Quantum Machine Learning strategies for accelerated drug discovery

As part of the Hartree National Centre for Digital Innovation, we worked with IBM to investigate the potential of quantum computing to accelerate the drug discovery process and reduce costs through Ligand-Based Virtual Screening, a computational technique that screens digital databases of molecules to identify structures most likely to bind to a drug target.

Our project showed that the Quantum Support Vector Classifier often performed better than an equivalent classical HPC algorithm and sometimes greatly outperformed the deep learning methodologies that are currently state of the art in drug discovery.

Training traditional machine learning algorithms can be prohibitively resource intensive, so quantum-enabled machine learning offered a potential advantage by supporting calculations at exponentially higher-orders of complexity to increase efficiency and accuracy. In February 2023, the team published a journal article on the results and are scoping potential follow-on projects with UK pharmaceutical companies.

This knowledge discovery saw a new concept and approach that integrates and applies quantum computing to drug discovery and life sciences.

Quantum

“

We are working flat out to explore quantum technology and its applications in various industries. Our efforts involve demystifying the technology through training and skills development. Additionally, we aim to de-risk investments in emerging technologies like quantum by delivering proof of concepts. These concepts will illustrate how quantum technology can effectively solve real-world challenges faced by industries. In our approach, we leverage multiple technologies, including classical high-performance computing (HPC), artificial intelligence (AI), and quantum technology. By combining these tools, we strive to provide practical solutions tailored to the needs of UK businesses.”



Stefano Mensa, Advanced Computing and Emerging Technologies Lead



Looking forward

“

As the Hartree Centre concludes another successful year, it remains focused on the future of digital and data driven technologies and, critically, their application to UK businesses and the public sector. This year I've been thrilled to see the centre expand its engagement with SMEs across the country through the establishment of three new regional hubs partnered with universities in Cardiff, the North East and Northern Ireland. The team continuously strives to enhance its digital innovation capabilities and knowledge, including into internationally emerging domains such as exascale and quantum computing.



What makes the Hartree Centre stand out is the continuous focus on how we will translate these emerging digital technologies to solve challenges and deliver meaningful societal and economic impact for UK industry. I'm excited to see what the Hartree Centre does next, and am confident that by fostering collaboration, driving investment decisions, and nurturing talent, the team is well-positioned to shape the future of digital innovation in the UK and beyond.”

Professor Mark Thomson, Executive Chair, Science and Technology Facilities Council (STFC)